Supplementary Information (SI) for Organic & Biomolecular Chemistry.
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Supporting Information

Asymmetric Synthesis of C–N Axially Chiral Carbazoles via Axial-to-Axial Chirality Transfer

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1. General Information and Materials

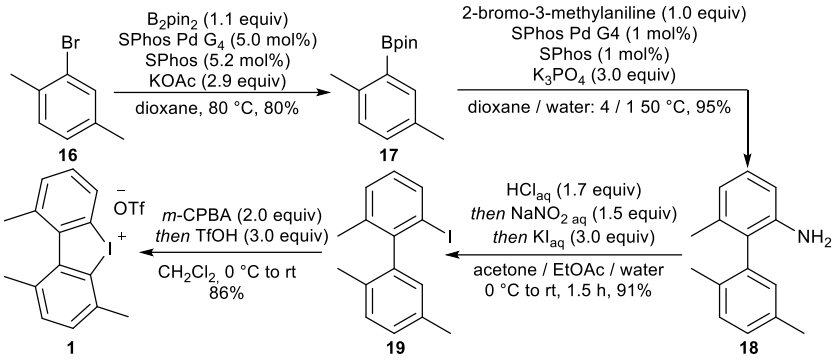
1.1 Chemicals

Chemicals were purchased from *Sigma-Aldrich Co.*, *Alfa Aesar GmbH & Co. KG*, *Merck KGaA* or *BLD Pharmatech GmbH* and used without further purification. Anhydrous dichloromethane, diethyl ether and tetrahydrofuran were taken from the solvent purifier *MB SPS-800* by *MBraun*. Silica gel 60 (0.040 – 0.063 mm, 230 – 400 mesh) for column chromatography was obtained from *Macherey Nagel*. Anhydrous solid reagents were stored in a desiccator under an atmosphere of N_2.

1.2 Analytical Equipment

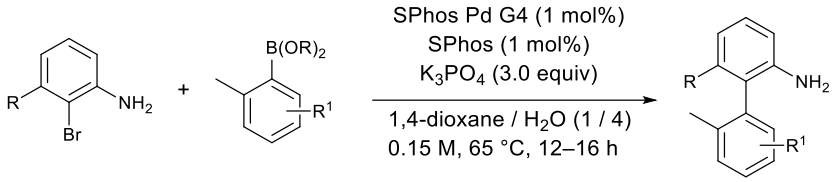
NMR spectra were measured on the spectrometer *Bruker Avance/DRX 600* at a frequency of 600 MHz (^{1}H) and 151 MHz (^{13}C) as well as *Bruker Avance/DRX 300* at a frequency of 282 MHz (^{19}F), 96 MHz (^{11}B), 300 MHz (^{1}H) and 75.5 MHz (^{13}C) in the indicated solvent. The ^{1}H- and ^{13}C-spectra were referenced to the solvent peak ($CDCl_3$ δ = 7.26 ppm (^{1}H), δ = 77.16 ppm (^{13}C)). Data were evaluated with *MNova* (*MestReNova*) version 14.1.2 by *Mestrelab Research*. Coupling constants *J* are given in Hz and chemical shifts δ in ppm (parts per million). Multiplicities are abbreviated as the following: singlet (s), broad singlet (brs), doublet (d), triplet (t), quartet (q), multiplet (m). Chiral HPLC analysis was performed using Dionex UltiMate 3000 from Thermo Scientific. ECD spectra were recorded on a Jasco J-1100 Circular Dichroism Spectrophotometer in a Quartz cuvette with 0.2 cm path length at 25 °C. The spectra were recorded in range of 185–400 nm in 0.5 nm increments with a scanning speed of 50 nm min^{-1} as an average of 16 spectra. Final concentrations were 100 µM in acetonitrile. High resolution mass spectrometry (HRMS) was measured at the Heinrich Heine University Düsseldorf (Applied Biosystems/ MDS SCIEXQ Model Trap 4000) with electron spray ionization (ESI). Low resolution mass spectrometry was conducted using the expression CMS system by Advion, Inc. in combination with an atmospheric pressure chemical ionization (APCI) or electron spray ionization (ESI). Gas chromatographic mass spectrometry (GC-MS(EI)) was conducted using the Thermo Scientific TRACE 1310 gas chromatograph (ISQ QD Single Quadrupole Mass Spectrometer, Helium). Optical rotation was measured with A.Krüss P8000-TF at 10 °C (c in g/100 ml). Melting points were measured with Stuart Scientific Melting Point Apparatus SMP3. IR spectra were recorded using the *SpectrumTwo FT-IR* by *PerkinElmer* with attenuated total reflection (ATR). The absorption bands are given in units of wave numbers (cm^{-1}). Elemental analysis was measured at the Heinrich Heine University Düsseldorf (Elementar, Vario Micro Cube).

2. Synthetic Procedures and Compound Characterization



Scheme 1: Exemplary synthesis overview towards diaryliodonium salts

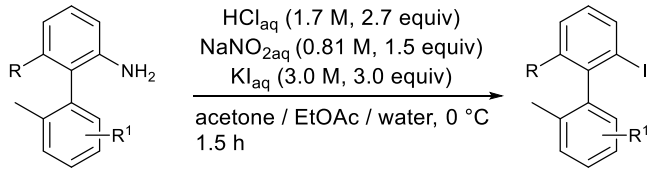
2.1 General Procedure A: Synthesis of 2-Aminobiarlys



A 10 ml flask was charged with 2-bromo-3-methylaniline (1.0 equiv) and closed with a rubber septum. The liquid was degassed in fine vacuum (< 10^{-2} mbar) for 30 minutes. Inert gas atmosphere (N_2) was applied. Water was degassed in a round bottom flask by combined Ar-purge and ultrasonication. The appropriate arylboronic acid (1.3 equiv), K_3PO_4 (3.0 equiv), SPhos Pd G4 (1 mol%) and SPhos (1 mol%) were weighed into a Schlenk flask containing a PTFE-coated magnetic stir bar and N_2-atmosphere applied. 2-bromo-3-methylaniline was dissolved in dioxane (0.15 M) and transferred to the Schlenk-flask. Water and if – necessary – dioxane was added to the Schlenk-flask to a final concentration of 0.15 M. The reaction mixture was heated in an oil bath to 65 °C and stirred at 750 rpm for 14 – 16 h.

After full consumption of starting material, the reaction was cooled to room temperature, diluted with EtOAc and filtered through silica. The solvent was removed *in vacuo*. The resulting crude product was purified via column chromatography on silica gel and petroleum ether / EtOAc mixtures as eluent.

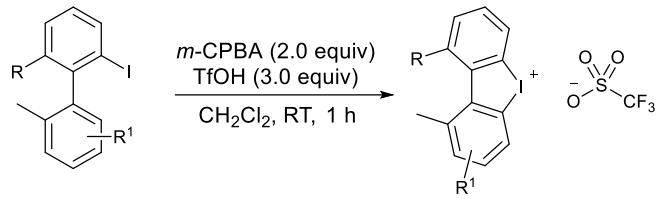
2.2 General Procedure B: Synthesis of 2-Iodobiaryls



In a round bottom flask 2-aminobiaryl was dissolved in acetone (1 M) and aqueous HCl (1.7 M, 2.7 equiv) was added in one portion. The solution was cooled to 0 °C and aqueous

$NaNO_2$ (0.81 M, 1.5 equiv) added. The solution was stirred for 30 minutes before the addition of EtOAc (1.0 equiv). Aqueous KI (3.0 equiv) was then added at 0 °C over 1 h using a syringe pump. After complete addition, the reaction was allowed to warm to room temperature and poured into a separatory funnel. The reaction mixture was washed twice with saturated, aqueous $Na_2S_2O_3$-solution, once with brine and then dried over $MgSO_4$. Following filtration, the solvent was removed *in vacuo*. The crude product was filtered with pentane through silica gel and not further purified.

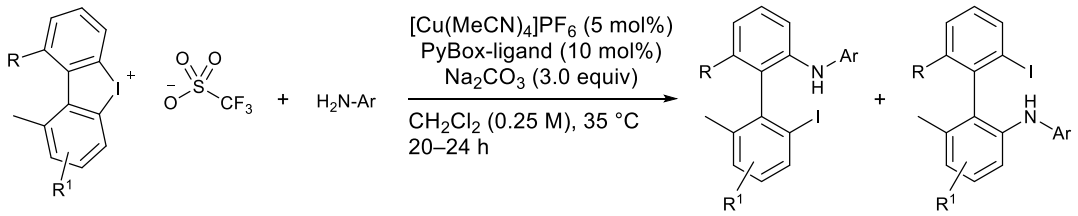
2.3 General Procedure C: Synthesis of Iodoniums Salts



In a round bottom flask equipped with a PTFE-coated magnetic stir bar, 2-iodobiaryl (1.0 equiv) was dissolved in dichloromethane (0.25 M). *m*-CPBA (2.0 equiv) was added in one portion. Once all solids had dissolved, the reaction mixture was cooled to 0 °C in an ice bath and TfOH (3.0 equiv) added dropwise over 1 min. The ice bath was removed and the reaction mixture stirred for 1 h. The solvent was then removed *in vacuo* and an equal amount of Et_2O added. The solids were dispersed in an ultrasonic bath and it was stirred at room temperature (RT) for 20 min. The precipitated product was obtained after filtration and washing with Et_2O.

For some derivatives it was found that increasing the amount of trifluoromethanesulfonic acid to 4.0 equivalents produced higher and more consistent yields. The corresponding reactions are labeled accordingly. No beneficial effects were observed from further increasing the equivalents.

2.4 General Procedure D: Synthesis of 2'-Amino-2-iodobiaryls

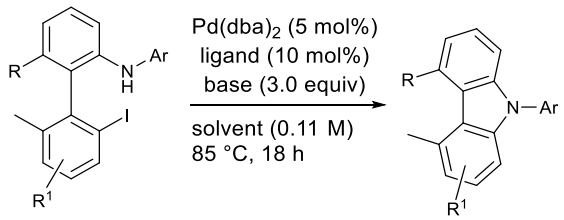


Iodonium salt (1.0 equiv), Na_2CO_3 (3.0 equiv), $[Cu(MeCN)_4]PF_6$ (5 mol%) and PyBox-ligand (10 mol%) were weighed into a round bottom flask equipped with a PTFE-coated magnetic stir bar and purged with argon for 10 min. Dichloromethane (0.05 M) was added and the reaction mixture stirred in an oil bath at 35 °C for 5 min. Arylamine was then added and the reaction stirred at 35 °C for 20–24 h.

Once all starting material was consumed, the reaction was allowed to cool to room temperature and filtered with dichloromethane through silica. Celite was added and the

solvent removed *in vacuo*. The product was isolated via column chromatography on silica using petroleum ether / EtOAc mixtures as eluent.

2.5 Synthesis of Carbazoles



General Procedure E: Screening of the reaction conditions of carbazole syntheses:

All screening reactions were performed on a 0.05 mmol scale. A stock solution of starting material (0.11 M) was prepared in the solvent used under inert atmosphere. Base, ligand and catalyst-precursor were weighed into an oven-dried 8 ml screw top reaction vessel containing a PTFE-coated magnetic stir bar and closed with a rubber septum. Between each weighing step, the reaction vessel was purged with argon-gas through a cannula. After addition of base, ligand and catalyst precursor the vessel was purged for 10 min with argon. The solution of starting material was added via syringe through the septum, which subsequently was exchanged for a screw cap fitted with a PTFE seal. The reaction was heated in an oil bath for 18 h and stirred at 750 rpm.

After 18 h the reaction was cooled to room temperature and filtered with 10 ml EtOAc through 1 ml silica in a 2 ml syringe. Solvent was removed *in vacuo* and 1,3,5-trimethoxybenzene (~5 mg) added as an internal NMR-standard. The yield was determined via ^{1}H-qNMR (D1 = 10 sec) in $CDCl_3$. The crude product was further purified via column chromatography using silica as stationary phase and a 98:2 mixture of petroleum ether and EtOAc as the eluent. The enantiomeric excess of the product was determined via chiral HPLC.

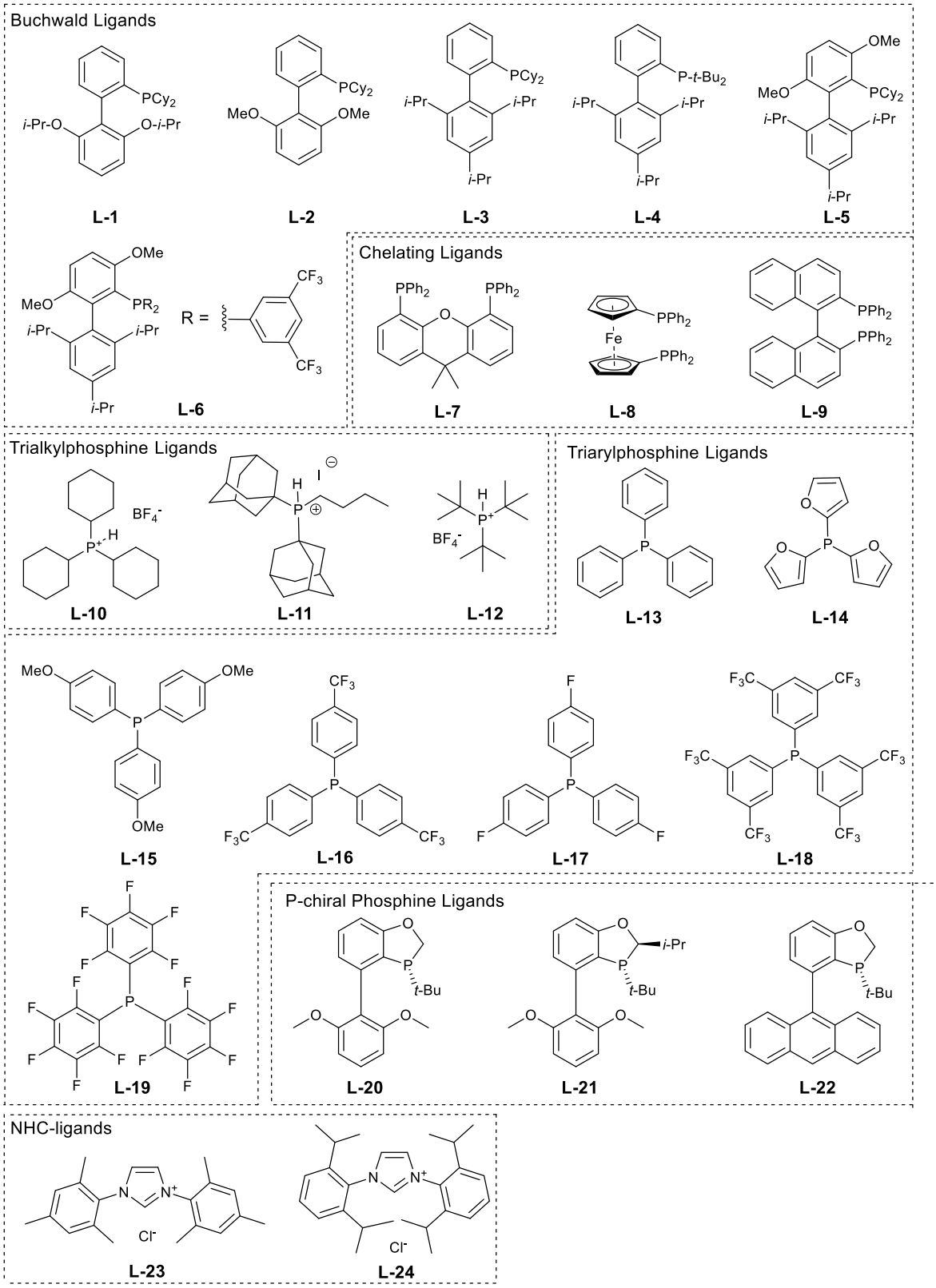


Figure S1: Screened ligands for the synthesis of carbazole **11**

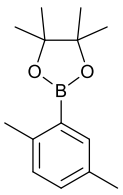
Table S1: Optimization of the synthesis of carbazole **11**. ee_{SMA}: enantiomeric excess of the starting material; conv.: conversion to product based on ^{1}H-qNMR with 1,3,5-trimethoxybenzene as internal standard; *ee*: enantiomeric excess of the product

#	Pd-source	Ligand	Solvent	Base	Temperature [°C]	ee_{SMA} [%]	conv. [%]	*ee* [%]
1	$Pd(dba)_2$	**L-1**	Glyme	K_3PO_4	85	92	72	75
2	$Pd(dba)_2$	**L-2**	Glyme	K_3PO_4	85	93	90	70
3	$Pd(dba)_2$	**L-3**	Glyme	K_3PO_4	85	92	65	40
4	$Pd(dba)_2$	**L-4**	Glyme	K_3PO_4	85	93	8	64
5	$Pd(dba)_2$	**L-5**	Glyme	K_3PO_4	85	92	68	58
6	$Pd(dba)_2$	**L-6**	Glyme	K_3PO_4	85	92	15	67
7	$Pd(dba)_2$	**L-7**	Glyme	K_3PO_4	85	89	75	63
8	$Pd(dba)_2$	**L-8**	Glyme	K_3PO_4	85	91	73	74
9	$Pd(dba)_2$	***rac*-L-9**	Glyme	K_3PO_4	85	89	56	76
10	$Pd(dba)_2$	**(*R*)-L-9**	Glyme	K_3PO_4	85	91	77	79
11	$Pd(dba)_2$	**(*S*)-L-9**	Glyme	K_3PO_4	85	91	87	79
12	$Pd(dba)_2$	**L-10**	Glyme	K_3PO_4	85	91	65	8
13	$Pd(dba)_2$	**L-11**	Glyme	K_3PO_4	85	93	81	3
14	$Pd(dba)_2$	**L-12**	Glyme	K_3PO_4	85	91	72	32
15	$Pd(dba)_2$	**L-13**	Glyme	K_3PO_4	85	91	60	37
16	$Pd(dba)_2$	**L-14**	Glyme	K_3PO_4	85	93	84	68
17	$Pd(dba)_2$	**L-15**	Glyme	K_3PO_4	85	91	53	40
18	$Pd(dba)_2$	**L-16**	Glyme	K_3PO_4	85	91	92	80
19	$Pd(dba)_2$	**L-17**	Glyme	K_3PO_4	85	91	68	68
20	$Pd(dba)_2$	**L-18**	Glyme	K_3PO_4	85	91	94	80
21	$Pd(dba)_2$	**L-19**	Glyme	K_3PO_4	85	89	9	75
22	$Pd(dba)_2$	**(*rac*)-L-20**	Glyme	K_3PO_4	85	91	49	47
23	$Pd(dba)_2$	**(*R*)-L-20**	Glyme	K_3PO_4	85	91	65	50
24	$Pd(dba)_2$	**(*R,R*)-L-21**	Glyme	K_3PO_4	85	91	20	62
25	$Pd(dba)_2$	**(*rac*)-L-22**	Glyme	K_3PO_4	85	91	80	62

26	$Pd(dba)_2$	**(*R*)-L-22**	Glyme	K_3PO_4	85	91	77	65
27	$Pd(dba)_2$	**L-23**	Glyme	K_3PO_4	85	91	36	40
28	$Pd(dba)_2$	**L-24**	Glyme	K_3PO_4	85	91	26	57
29	$Pd(dba)_2$	**L-1**	Glyme	K_3PO_4	75	92	69	78
30	$Pd(dba)_2$	**L-1**	Glyme	K_3PO_4	70	92	67	76
31	$Pd(dba)_2$	**L-1**	Glyme	K_3PO_4	65	92	51	79
32	$Pd(dba)_2$	**L-1**	THF	K_3PO_4	65	91	4	—
33	$Pd(dba)_2$	**L-1**	1,4-dioxane	K_3PO_4	65	91	62	76
34	$Pd(dba)_2$	**L-1**	Toluene	K_3PO_4	65	91	69	76
35	$Pd(dba)_2$	**L-1**	DMF	K_3PO_4	65	91	53	75
36	$Pd(dba)_2$	**L-1**	*t*-BuOH	K_3PO_4	65	91	77	79
37	$Pd(dba)_2$	**L-1**	DMF	*t*-BuOK	65	91	87	77
38	$Pd(dba)_2$	**L-1**	*t*-BuOH	Cs_2CO_3	65	91	82	78
39	$Pd(dba)_2$	**L-16**	*t*-BuOH	*t*-BuOK	65	91	74	74
41	$Pd(dba)_2$	**L-16**	Glyme	*t*-BuOK	65	91	84	82
42	$Pd(dba)_2$	**L-16**	*t*-BuOH	K_3PO_4	65	91	81	70
43	$Pd(dba)_2$	**L-16**	Toluene	*t*-BuOK	65	91	96	13
44	$Pd(dba)_2$	**L-16**	1,4-dioxane	*t*-BuOK	65	91	45	49
45	$Pd(dba)_2$	**L-16**	DMF	*t*-BuOK	65	91	96	80

General Procedure E: optimized carbazole synthesis:

2-(2,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (17)



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SPhos (74.5 mg, 3.0 mol%), SPhos Pd G4 (142.5 mg, 3.0 mol%), bis(pinacolato)diboron (1.68 g, 1.1 equiv) and potassium acetate (1.77 g, 3.0 equiv) were degassed in a Schlenk-tube containing a PTFE-coated, magnetic stir bar and 15 ml 1,4-dioxane added. 830 µL 2-bromo-1,4-dimethylbenzene were degassed under vacuum in a separate vial and transferred with

5 ml 1,4-dioxane to the reaction vessel. The reaction mixture was stirred at 80 °C under nitrogen atmosphere for 15 h. The reaction mixture was subsequently filtered through celite with EtOAc, washed with aqueous, saturated $NaHCO_3$ and brine. The organic phases were dried over $MgSO_4$, filtered and the solvent removed *in vacuo*. 1.11 g of the title compound (4.77 mmol, 80%) were obtained after column chromatography on silica gel as a faint yellow oil (petroleum ether / ethyl acetate = 98/2).

The reaction was repeated in scales of 0.54 mmol to 3.0 mmol with yields ranging from 57% to 83%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.58 (d, *J* = 2.1 Hz, 1H), 7.15 – 7.11 (m, 1H), 7.06 (d, *J* = 7.7 Hz, 1H), 2.49 (s, 3H), 2.31 (s, 3H), 1.34 (s, 12H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 141.73, 136.36, 133.94, 131.57, 129.81, 83.37, 24.90, 21.73, 20.81

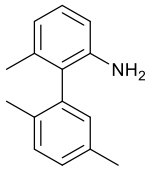
^{11}B NMR (96 MHz, $CDCl_3$) δ 30.98

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2977, 1403, 1341, 1306, 1143, 1069, 855, 813, 733, 665, 516

MS (EI): *m/z* 232.20

The analytical data are in accordance with those reported in literature.[1] Due to spin coupling between carbon and boron, the aromatic carbon atom carrying the Bpin-substituent is not visible in the ^{13}C NMR spectrum.

2',5',6-trimethyl-[1,1'-biphenyl]-2-amine (18)



18

The reaction was performed following general procedure A. 619 mg 2-bromo-3-methylaniline (3.33 mmol, 1.0 equiv) were reacted with 994 mg 2-(2,5-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.28 mmol, 1.3 equiv). 672 mg of the title compound (3.18 mmol, 95%) were obtained as a faint yellow oil after column chromathography on silica gel (petroleum ether / ethyl acetate: 97/3).

The reaction was repeated in scales of 0.54 mmol to 3.3 mmol with yields ranging from 84% to 94%.

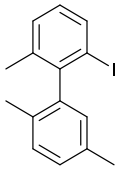
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.20 (d, *J* = 7.7 Hz, 1H), 7.10 – 7.05 (m, 2H), 6.93 (s, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 6.68 (d, *J* = 8.2 Hz, 1H), 3.73 (bs, 2H), 2.32 (s, 3H), 2.02 (s, 3H), 1.93 (s, 3H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 143.31, 137.26, 136.98, 136.09, 133.88, 130.51, 130.45, 128.51, 127.87, 127.69, 120.30, 112.95, 21.11, 20.33, 18.93.

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3376, 2919, 1608, 1580, 1468, 1303, 1032, 810, 779, 754, 478

The analytical data are in accordance with those reported in literature.[2]

2'-iodo-2,5,6'-trimethyl-1,1'-biphenyl (19)



19

The reaction was performed following general procedure B. Starting from 660 mg 2',5',6-trimethyl-[1,1'-biphenyl]-2-amine (3.12 mmol, 1.0 equiv), 916 mg of the title compound were obtained as a faint yellow oil (2.84 mmol, 91%).

The reaction was repeated in scales of 0.47 mmol to 3.08 mmol with yields ranging from 70% to 86%.

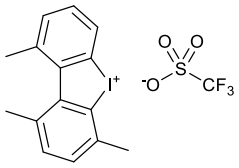
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.77 (d, *J* = 7.9 Hz, 1H), 7.23 (dt, *J* = 7.5, 1.0 Hz, 1H), 7.17 (d, *J* = 7.7 Hz, 1H), 7.11 (dd, *J* = 7.8, 1.9 Hz, 1H), 6.94 (t, *J* = 7.7 Hz, 1H), 6.81 – 6.78 (m, 1H), 2.35 (s, 3H), 2.03 (s, 3H), 1.95 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 146.1, 143.9, 137.8, 136.5, 135.6, 132.3, 130.0, 129.8, 129.4, 128.9, 128.6, 101.2, 22.0, 21.2, 19.1

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2918, 1553, 1500, 1440, 1171, 1121, 809, 766, 651, 470

HRMS (ESI): m/z = calcd for $[C_{14}H_{14}I + H]^+$: 321.0135 found 321.0136

1,4,9-trimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (1)



1

The reaction was performed following general procedure C. Starting from 916 mg 2'-iodo-2,5,6'-trimethyl-1,1'-biphenyl (2.84 mmol, 1.0 equiv), 1.14 g of the title compound (2.43 mmol, 86%) were obtained as a beige solid after column chromatography (petroleum ether / ethyl acetate: 10/90).

The reaction was repeated in scales of 0.33 mmol to 2.66 mmol with yields ranging from 65% to 75%.

^{1}H NMR (300 MHz, $CDCl_3$) δ 8.27 (d, *J* = 8.2 Hz, 1H), 7.67-7.4f7 (m, 3H), 7.40 (d, *J* = 7.8 Hz, 1H), 2.65 (s, 3H), 2.56 (s, 3H), 2.52 (s, 3H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 142.53, 141.61, 138.61, 135.61, 135.01, 134.52, 130.49, 130.44, 129.08, 123.49, 120.44 (q, J_{C-F} = 319.6 Hz) 120.38, 26.06, 24.12, 23.73

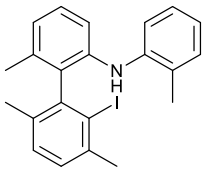
^{19}F NMR (282 MHz, $CDCl_3$) δ -78.08

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 1736, 1441, 1278, 1232, 1159, 1025, 823, 776, 635, 574, 516

mp 143 °C (from Et_2O)

The analytical data are in accordance with those reported in literature.[2]

2'-iodo-3',6,6'-trimethyl-N-(o-tolyl)-[1,1'-biphenyl]-2-amine (2)



2

The reaction was performed following general procedure D with the following exceptions: No chiral ligand and 10 mol% $[Cu(MeCN)_4]PF_6$ were used. 151 mg 1,4,9-trimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.32 mmol, 1.0 equiv) were reacted with 41 mg *o*-toluidine (0.38 mmol, 1.2 equiv). 103.2 mg of the racemic title compound (0.24 mmol, 75%) were obtained as a faint yellow oil after column chromatography on silica gel (petroleum ether / ethyl acetate: 98/2).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.27 (dd, *J* = 8.5, 1.4 Hz, 1H), 7.21 – 7.15 (m, 3H), 7.12 (td, *J* = 6.8, 6.1, 1.6 Hz, 2H), 6.92 (td, *J* = 7.4, 1.3 Hz, 1H), 6.88 (d, *J* = 8.2 Hz, 1H), 6.83 – 6.79 (m, 1H), 2.51 (s, 3H), 2.08 (s, 3H), 2.02 (s, 3H), 1.92 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 142.6, 141.2, 140.8, 140.7, 136.5, 135.9, 132.6, 130.9, 130.3, 130.2, 129.1, 128.3, 126.8, 122.7, 121.1, 121.0, 112.1, 109.1, 29.7, 21.1, 19.9, 17.8

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2922, 1751, 1461, 1366, 1195, 1022, 867, 812, 803, 785, 747

HRMS (ESI): m/z = calcd for $[C_{22}H_{22}IN + H]^+$: 428.0870 found: 428.0870

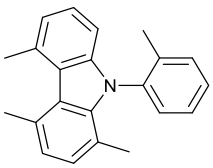
Enantiomer 1:

$[\alpha]_D^{20}$: -64.7° (c = 0.47, $CHCl_3$)

Enantiomer 2:

$[\alpha]_D^{20}$: 147.9° (c = 0.43, $CHCl_3$)

1,4,5-trimethyl-9-(o-tolyl)-9H-carbazole (4)



4

The reaction was performed following general procedure E under the optimized conditions (see Table S1, entry 18). Starting from 47.3 mg 2'-iodo-3',6,6'-trimethyl-N-(o-tolyl)-[1,1'-biphenyl]-2-amine (0.11 mmol, 1.0 equiv), 29.5 mg of the title compound (0.099 mmol, 89%) were obtained as a faint yellow oil after column chromatography on silica gel (petroleum ether / ethyl acetate: 99/1).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.44 (td, *J* = 7.4, 1.7 Hz, 1H), 7.39 (d, 1H, *J* = 7.47 Hz), 7.37 – 7.31 (m, 2H), 7.21 (dd, *J* = 8.2, 7.2 Hz, 1H), 7.04 (m, *J* = 7.11 Hz, 2H), 6.96 (d, *J* = 7.3 Hz, 1H), 6.69 (d, *J* = 8.1 Hz, 1H), 3.07 (s, 3H), 3.05 (s, 3H), 1.91 (s, 3H), 1.90 (s, 3H)

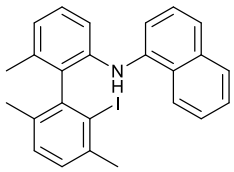
^{13}C NMR (151 MHz, $CDCl_3$) δ 142.90, 139.84, 139.09, 138.53, 132.10, 130.71, 130.55, 130.06, 129.02, 128.56, 126.82, 125.49, 123.51, 123.31, 123.00, 122.53, 118.54, 108.05, 26.50, 26.23, 19.16, 17.45

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2925, 1576, 1496, 1452, 1374, 1304, 1259, 1126, 798, 752

HRMS (ESI): m/z = calcd for $[C_{22}H_{21}N + H]^+$: 300.1747 found: 300.1750

$[\alpha]_D^{20}$: -12.0° (c = 0.54, $CHCl_3$, 71% *ee*)

N-(2'-iodo-3',6,6'-trimethyl-[1,1'-biphenyl]-2-yl)naphthalen-1-amine (3)



3

The reaction was performed following general procedure D. 150 mg 1,4,9-trimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.32 mmol, 1.0 equiv) were reacted with 54.8 mg 1-naphthylamine (0.38 mmol, 1.2 equiv) yielding 108 mg of the title compound (0.23 mmol, 72%, 92%*ee*) as an orange solid.

The reaction was repeated at scales of 0.11 mmol and 0.21 mmol with yields of 57% and 66% respectively.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.4 Hz, 1H), 7.85 – 7.81 (m, 1H), 7.58 (d, *J* = 8.0 Hz, 1H), 7.50 – 7.36 (m, 4H), 7.25 (d, *J* = 7.7 Hz, 1H), 7.20 (d, *J* = 7.7 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 1H), 6.84 (dd, *J* = 7.9, 2.9 Hz, 2H), 5.27 (s, 1H), 2.55 (s, 3H), 2.21 (s, 3H), 1.97 (s, 3H)

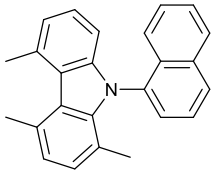
^{13}C NMR (151 MHz, $CDCl_3$) δ 142.52, 142.21, 140.94, 138.49, 136.47, 135.96, 134.74, 132.39, 130.47, 129.33, 129.07, 128.48, 128.29, 126.15, 126.14, 125.79, 123.81, 122.52, 121.18, 118.71, 112.48, 109.27, 29.70, 21.26, 20.00

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3391, 2918, 1574, 1519, 1496, 1465, 1399, 1306, 1094, 780,

HRMS (ESI): m/z = calcd.: $C_{25}H_{23}IN$: $[M+H]^+$ = 464.0870; found: 464.0876

$[\alpha]_D^{20}$: -101.6° (c = 0.38, $CHCl_3$)

1,4,5-trimethyl-9-(naphthalen-1-yl)-9H-carbazole (5)



5

The reaction was performed following general procedure E under the optimized conditions (see Table S1, entry 18). Starting from 34.4 mg racemic N-(2'-iodo-3',6,6'-trimethyl-[1,1'-biphenyl]-2-yl)naphthalen-1-amine (0.074 mmol, 1.0 equiv), 24.3 mg of the title compound (0.072 mmol, 97%, 60%*ee*) were obtained as an orange solid after column chromatography on silica gel (petroleum ether / ethyl acetate: 99/1).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.05 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.99 (d, *J* = 8.3 Hz, 1H), 7.62 (dd, *J* = 8.2, 7.1 Hz, 1H), 7.59 (s, 1H), 7.52 (ddd, *J* = 8.1, 6.7, 1.2 Hz, 1H), 7.31 (ddd, *J* = 8.2, 6.7, 1.2 Hz, 1H), 7.20 – 7.16 (m, 1H), 7.14 (t, *J* = 7.7 Hz, 1H), 7.05 (d, *J* = 7.1 Hz, 1H), 7.00 (s, 2H), 6.62 (d, *J* = 8.1 Hz, 1H), 3.11 (d, *J* = 7.0 Hz, 6H), 1.69 (s, 3H)

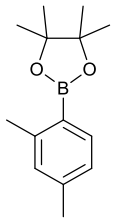
^{13}C NMR (151 MHz, $CDCl_3$) δ 144.14, 141.01, 136.90, 134.18, 132.86, 132.08, 130.08, 129.23, 128.65, 128.40, 128.11, 127.46, 126.82, 125.53 (d, *J* = 4.5 Hz), 123.69, 123.48, 123.24, 122.59, 118.82, 108.52, 26.54, 26.27, 25.03, 19.18

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2922, 1597, 1573, 1451, 1421, 1301, 1258, 1125, 780, 704, 631, 552

HRMS (ESI): m/z = calcd for $[C_{25}H_{21}N + H]^+$: 336.1747 found: 336.1746

$[\alpha]_D^{20}$: -2.2° (c = 0.45, $CHCl_3$)

2-(2,4-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (20)



20

SPhos (62.0 mg, 2.5 mol%) and SPhos Pd G4 (120.1 mg, 2.5 mol%) were degassed in a Schlenk-tube closed with a rubber septum and containing a PTFE-coated, magnetic stir bar and dissolved in 10 ml 1,4-dioxane. 1-bromo-2,4-dimethylbenzene (810 µL, 6.0 mmol) was degassed in an oven dried round bottom flask, dissolved in 10 ml 1,4-dioxane and transferred via syringe to the catalyst containing Schlenk-tube. The mixture was stirred and heated to 65 °C and pinacolborane (1.3 mL, 1.5 equiv) added via syringe. After stirring for 10 min triethylamine (2.5 ml, 3.0 equiv) was added via syringe and the reaction stirred at 65 °C for 17 h. Workup was performed by filtration of the reaction mixture through silica with ethyl

acetate. The solvent was removed *in vacuo* the product isolated via column chromatography on silica gel (petroleum ether / ethyl acetate = 97/3). The product was obtained as a colourless oil (1.25 g, 90%).

The reaction was repeated in scales of 3.0 mmol to 6.0 mmol with yields ranging from 85% to 96%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 (d, *J* = 7.4 Hz, 1H), 7.29 (s, 0H), 7.04 – 6.99 (m, 2H), 2.53 (s, 3H), 2.34 (s, 3H), 1.36 (s, 12H)

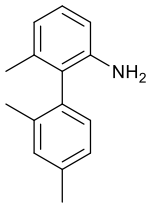
^{13}C NMR (151 MHz, $CDCl_3$) δ 144.95, 140.87, 136.10, 130.73, 125.54, 83.24, 24.89, 22.12, 21.50

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2977, 1611, 1372, 1342, 1309, 1272, 1145, 1132, 1062, 963, 859, 819, 658

MS (EI): *m/z* 232.38

The analytical data are in accordance with those reported in literature.[1]

2',4',6-trimethyl-[1,1'-biphenyl]-2-amine (21)



21

The reaction was performed following general procedure A. 569 mg 2-bromo-3-methylaniline (3.06 mmol, 1.0 equiv) were reacted with 1.18 g 2-(2,4-dimethylphenyl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane (4.58 mmol, 1.5 equiv) yielding 610 mg of the title compound (2.89 mmol, 94 %) as a yellow oil. A catalyst loading of 4 mol% was used in this reaction.

The reaction was repeated once at the same scale with a yield of 94%. Performing the reaction at a lower temperature of 50°C resulted in decreased yields of 51% (0.65 mmol scale) to 57% (1.46 mmol scale).

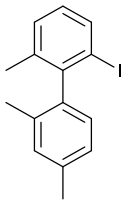
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.15 (s, 1H), 7.11 – 7.04 (m, 2H), 7.00 (d, *J* = 7.6 Hz, 1H), 6.71 (d, *J* = 7.5 Hz, 1H), 6.64 (d, *J* = 7.9 Hz, 1H), 3.31 (s, 3H), 2.37 (s, 3H), 2.04 (s, 3H), 1.93 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 144.08, 137.30, 137.18, 136.97, 134.51, 131.38, 129.87, 127.87, 127.46, 127.21, 119.92, 112.60, 21.32, 20.37, 19.34

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3468, 3376, 2919, 1607, 1579, 1463, 1302, 1004, 820, 776, 745, 579

HRMS (ESI): m/z = calcd for $[C_{15}H_{17}N + H]^+$: 212.1434 found 212.1433

2'-Iodo-2,4,6'-trimethyl-1,1'-biphenyl (22)



22

The reaction was performed following general procedure B. Starting from 600 mg 2',4',6-trimethyl-[1,1'-biphenyl]-2-amine (2.84 mmol, 1.0 equiv) 848 mg of the title compound (2.63 mmol, 93 %) were obtained as a colourless oil.

The reaction was repeated at scales between 0.95 mmol and 2.79 mmol with yields ranging from 82% to 99%.

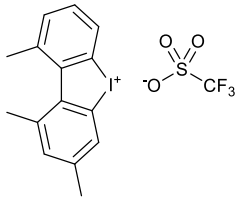
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.80 (d, *J* = 7.9 Hz, 1H), 7.26 (d, *J* = 7.6 Hz, 1H), 7.14 (s, 1H), 7.11 (d, 1H), 6.96 (t, *J* = 7.7 Hz, 1H), 6.89 (d, *J* = 7.6 Hz, 1H), 2.42 (s, 3H), 2.05 (s, 3H), 1.99 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.85, 141.07, 137.91, 137.41, 136.37, 135.09, 130.87, 129.66, 128.76, 128.57, 126.82, 101.52, 21.85, 21.32, 19.43

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2918, 1615, 1553, 1440, 1377, 1232, 1173, 1121, 1008, 812, 767, 575

MS (EI): *m/z* 322.14

1,3,9-Trimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (6)



6

The reaction was performed following general procedure C. Starting from 847 mg 2'-iodo-2,4,6'-trimethyl-1,1'-biphenyl (2.63 mmol, 1.0 equiv) 1.02 g of the title compound (2.16 mmol, 82%) were obtained as a beige solid.

The reaction was repeated at scales between 0.31 mmol and 1.87 mmol with yields ranging from 77% to 90%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (d, *J* = 8.0 Hz, 1H), 7.99 (d, *J* = 1.5 Hz, 1H), 7.48 (d, *J* = 7.5 Hz, 1H), 7.42 (t, *J* = 7.8 Hz, 1H), 7.29 (s, 1H), 2.48 (s, 3H), 2.46 (s, 3H), 2.41 (s, 3H).

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 141.97, 141.42, 139.98, 139.86, 139.36, 134.90, 133.86, 129.85, 129.26, 128.87, 122.3 (q, $J_{C\text{-}F}$ = 319.8 Hz), 120.21, 119.90, 24.13, 24.00, 21.22

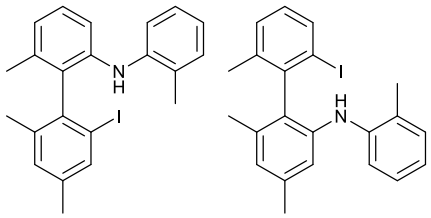
^{19}F NMR (282 MHz, $CDCl_3$) δ -78.00

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 1444, 1286, 1233, 1164, 1025, 776, 636, 517

Elemental analysis: Found: C, 40.5; H, 3.3; S, 6.9. Calc. for $C_{15}H_{14}I * CF_3O_3S$: C, 40.5; H, 3.0; S, 6.8

mp 197 °C (from Et_2O)

2'-Iodo-4',6,6'-trimethyl-N-(o-tolyl)-[1,1'-biphenyl]-2-amine (23a) & 2'-iodo-4,6,6'-trimethyl-N-(o-tolyl)-[1,1'-biphenyl]-2-amine (23b)

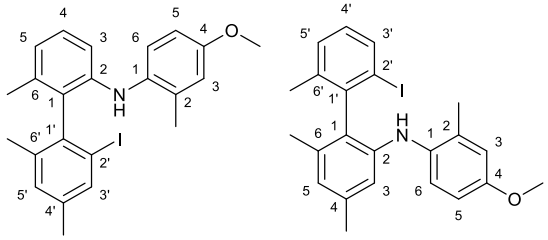


23a **23b**

The reaction was performed following general procedure D. 107 mg 1,3,9-trimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.23 mmol, 1.0 equiv) were reacted with 29.2 mg *o*-toluidine (0.27 mmol, 1.2 equiv) yielding 63 mg of an inseparable mixture of regioisomers A and B (total amount: 0.15 mmol, conversion to regioisomers: 64%) in a ratio of 59:41 (**23a**:**23b**).

2'-Iodo-N-(4-methoxy-2-methylphenyl)-4',6,6'-trimethyl-[1,1'-biphenyl]-2-amine (7a) &

2'-Iodo-N-(4-methoxy-2-methylphenyl)-4,6,6'-trimethyl-[1,1'-biphenyl]-2-amine (7b)



7a **7b**

The reaction was performed following general procedure D. 150 mg 1,3,9-trimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate were reacted with 52.9 mg 4-methoxy-2-methylaniline yielding 115 mg of regioisomers **7a** and **7b** in a 55:45 ratio (total amount: 0.25 mmol, conversion to regioisomers: 79%) after column chromatography on silica gel (petroleum ether / ethyl acetate: 98/2). 11.9 mg of title compound **7a** (0.03 mmol, 8%, 95%*ee*) and 38.2 mg of the title compound **7b** (0.84 mmol, 26 %, 95%*ee*) were isolated after preparative HPLC.

7a:

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.70 (s, 1H), 7.14 (s, 1H), 7.09 (t, *J* = 8.7 Hz, 2H), 6.74 (d, *J* = 2.9 Hz, 1H), 6.72 – 6.67 (m, 2H), 6.44 (d, *J* = 8.2 Hz, 1H), 4.59 (s, 1H), 3.78 (s, 4H), 2.32 (s, 3H), 2.12 (d, *J* = 7.9 Hz, 6H), 1.92 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 156.74, 143.37, 139.58, 138.97, 138.90, 137.94, 136.52, 135.53, 133.25, 131.63, 129.70, 128.40, 126.76, 119.70, 116.11, 112.04, 110.05, 102.56, 55.56, 21.34, 20.72, 20.00, 18.43

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3393, 2922, 1584, 1503, 1465, 1289, 1222, 1154, 1049, 854, 772

HRMS (ESI): m/z = calcd for $[C_{23}H_{24}INO + H]^+$: 458.0975 found 458.0979

$[\alpha]_D^{20}$: -61.7 (c = 0.54, $CHCl_3$)

7b:

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.9 Hz, 1H), 7.31 (d, *J* = 7.5 Hz, 1H), 7.12 (d, *J* = 8.6 Hz, 1H), 6.99 (t, *J* = 7.7 Hz, 1H), 6.76 (d, *J* = 3.0 Hz, 1H), 6.72 (dd, *J* = 8.6, 3.0 Hz, 1H), 6.57 (s, 1H), 6.31 (s, 1H), 4.94 – 4.00 (bs, 1H), 3.79 (s, 3H), 2.25 (s, 3H), 2.17 (s, 3H), 2.13 (s, 3H), 1.89 (s, 3H)

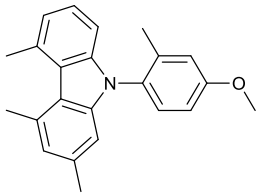
^{13}C NMR (151 MHz, $CDCl_3$) δ 156.62, 142.81, 142.28, 139.69, 138.32, 137.39, 135.93, 135.28, 133.29, 130.52, 129.54, 127.33, 126.54, 120.89, 116.13, 112.02, 110.93, 103.18, 55.55, 21.88, 21.52, 19.84, 18.42

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3397, 2916, 1733, 1575, 1500, 1440, 1229, 1160, 1053, 824, 771

HRMS (ESI): m/z = calcd for $[C_{23}H_{24}INO + H]^+$: 458.0975 found 458.0981

$[\alpha]_D^{20}$: -80.5 (c = 0.40, $CHCl_3$)

9-(4-Methoxy-2-methylphenyl)-2,4,5-trimethyl-9H-carbazole (8)



8

The reaction was performed following general procedure E under the optimized conditions (see Table S1, entry 18). Starting from 31.0 mg 2'-iodo-N-(4-methoxy-2-methylphenyl)-4',6,6'-trimethyl-[1,1'-biphenyl]-2-amine (0.07 mmol, 1.0 equiv, 83%*ee*) 24.1 mg of the title compound (0.07 mmol, >99%, 55%*ee*) were obtained.

Employing RuPhos as the ligand delivered the title compound with 73%*ee*, starting from 95%*ee* in the starting material.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.23 - 7.18 (m, 2H), 7.01 (d, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 2.9 Hz, 1H), 6.92 (dd, *J* = 8.5, 2.9 Hz, 1H), 6.87 (s, 1H), 6.80 (d, *J* = 8.1 Hz, 1H), 6.62 (s, 1H), 3.91 (s, 3H), 3.06 (s, 3H), 3.04 (s, 3H), 2.39 (s, 3H), 1.88 (s, 3H)

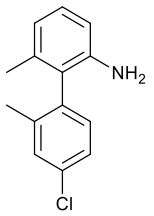
^{13}C NMR (151 MHz, $CDCl_3$) δ 159.73, 142.85, 142.33, 139.26, 135.74, 131.93, 131.88, 130.76, 129.08, 125.09, 124.68, 122.83, 122.61, 120.27, 116.54, 112.60, 107.84, 107.74, 55.63, 26.17, 26.11, 21.60, 17.85

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2924, 1596, 1505, 1447, 1310, 1231, 1158, 1053, 1031, 832, 762, 727

HRMS (ESI): m/z = calcd for $[C_{23}H_{23}NO + H]^+$: 330.1852 found 330.1849

$[\alpha]_D^{20}$: -9.2° (c = 0.51, $CHCl_3$, 69% *ee*)

4'-Chloro-2',6-dimethyl-[1,1'-biphenyl]-2-amine (24)



24

The reaction was performed following general procedure A. 932 mg 2-bromo-3-methylaniline (5.0 mmol, 1.0 equiv) were reacted with 852 mg (4-chloro-2-methylphenyl)boronic acid (5.0 mmol, 1.0 equiv). As side products, the coupling products of the title compound with unreacted (4-chloro-2-methylphenyl)boronic acid (and higher order coupling products) were formed, which were only partially separable from the title compound. 821 mg of the title compound (3.54 mmol, 71%) were obtained as a yellow oil after performing 3 repetitive isolations via column chromatography on silica gel (petroleum ether / ethyl acetate = 95/5).

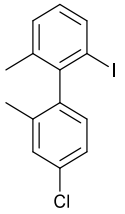
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.33 (d, *J* = 2.2 Hz, 1H), 7.28 – 7.23 (m, 2H), 7.10 (t, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 8.1 Hz, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 6.67 (d, *J* = 8.0 Hz, 1H), 4.40 – 3.14 (bs, 2H), 2.05 (s, 3H), 1.91 (s, 3H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 143.68, 139.40, 136.91, 136.06, 133.36, 131.40, 130.57, 128.32, 126.91, 125.82, 120.10, 112.80, 20.28, 19.33

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3380, 2921, 1610, 1590, 1465, 1304, 1195, 1096, 1004, 871, 822, 777, 745

HRMS (ESI): m/z = calcd for $[C_{14}H_{14}ClN + H]^+$: 232.0888 found: 232.0891

4-chloro-2'-iodo-2,6'-dimethyl-1,1'-biphenyl (25)



25

The reaction was performed following general procedure B. Starting from 2.05 g 4'-chloro-2',6-dimethyl-[1,1'-biphenyl]-2-amine (8.85 mmol, 1.0 equiv) 2.83 g of the title compound (8.28 mmol, 94 %) were obtained as a colourless oil.

The reaction was repeated at scales between 0.33 mmol and 6.9 mmol with yields ranging from 88% to 95%.

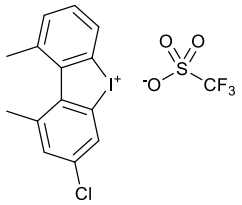
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 (d, *J* = 2.2 Hz, 1H), 7.28 (d, *J* = 10.1 Hz, 2H), 7.12 (t, *J* = 7.8 Hz, 1H), 7.09 (d, *J* = 8.1 Hz, 1H), 6.77 (d, *J* = 7.5 Hz, 1H), 6.71 (d, *J* = 8.0 Hz, 1H), 2.07 (s, 3H), 1.94 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 139.30, 136.94, 133.34, 131.31, 130.48, 128.27, 126.79, 20.15, 19.27

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2922, 1596, 1551, 1488, 1441, 1198, 1120, 1097, 1008, 872, 814, 769

MS (EI): *m/z* 231.13

3-Chloro-1,9-dimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (9)



9

The reaction was performed following general procedure C with the exception that 4.0 equivalents of trifluoromethanesulfonic acid were used. Starting from 508 mg 4-chloro-2'-iodo-2,6'-dimethyl-1,1'-biphenyl (1.48 mmol, 1.0 equiv), 517 mg of the title compound (1.05 mmol, 71%) were obtained as a beige solid.

The reaction was repeated twice at the same scale with yields of 65% and 68% respectively. Employing 3.0 equivalents of TfOH generally produced lower and inconsistent yields ranging between 16% and 44% at various scales. Increasing the amount of TfOH to 5.0 equivalents did not provide any additional benefit (0.95 mmol, 68% yield).

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 – 8.23 (m, 2H), 7.60 – 7.52 (m, 3H), 2.55 (d, *J* = 2.2 Hz, 6H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 140.82, 140.74, 140.33, 135.90, 134.08, 130.48, 128.86, 128.57, 120.62, 120.47, 120.38 (q, J_{C-F} = 319.2 Hz), 24.08, 23.95

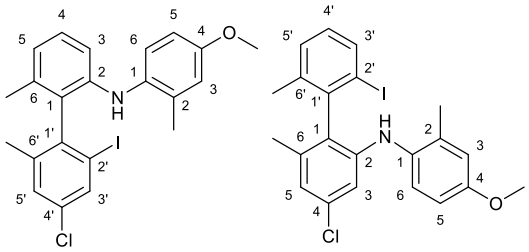
^{19}F NMR (282 MHz, $CDCl_3$) δ -77.98

mp 198 °C (from Et_2O)

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2922, 1739, 1439, 1371, 1274, 1218, 1161, 1023, 636, 515

HRMS (ESI): m/z = calcd for $[C_{14}H_{11}ClI]^+$: 340.9589 found: 340.9589

4'-Chloro-2'-iodo-N-(4-methoxy-2-methylphenyl)-6,6'-dimethyl-[1,1'-biphenyl]-2-amine (10a) & 4-chloro-2'-iodo-N-(4-methoxy-2-methylphenyl)-6,6'-dimethyl-[1,1'-biphenyl]-2-amine (10b)



10a **10b**

The reaction was performed following general procedure D. Starting from 599 mg 3-chloro-1,9-dimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (1.22 mmol, 1.0 equiv), 216 mg of title compound **10a** (0.45 mmol, 37%) and 89 mg of title compound **10b** (0.19 mmol, 15%) were obtained after column chromatography on silica gel (petroleum ether / ethyl acetate = 97 / 3). 30.3 mg were obtained as a 96:4 mixture of compounds **10b** and **10a**.

10a:

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (d, *J* = 2.1 Hz, 1H), 7.35 (d, *J* = 2.1 Hz, 1H), 7.12 – 7.05 (m, 2H), 6.76 (d, *J* = 2.9 Hz, 1H), 6.73 (s, 0H), 6.43 (d, *J* = 8.2 Hz, 1H), 4.50 (s, 1H), 3.78 (s, 3H), 2.14 (d, *J* = 6.3 Hz, 6H), 1.91 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 156.95, 143.22, 140.86, 140.61, 136.82, 136.26, 135.67, 134.16, 132.89, 130.75, 128.86, 128.58, 127.00, 119.91, 116.16, 112.14, 110.29, 102.65, 55.56, 21.42, 19.92, 18.44

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] =3401, 2922, 1576, 1508, 1422, 1296, 1223, 1049, 877, 772

HRMS (ESI): m/z = calcd for $[C_{22}H_{22}ClINO + H]^+$: 478.0429 found 478.0434

$[\alpha]_D^{20}$: -71.7 (c = 0.57, $CHCl_3$)

10b:

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 8.6 Hz, 1H), 7.01 (t, *J* = 7.8 Hz, 1H), 6.76 (d, *J* = 3.0 Hz, 1H), 6.72 (dd, *J* = 8.6, 3.0 Hz, 1H), 6.70 (d,

J = 2.0 Hz, 1H), 6.36 (d, *J* = 2.1 Hz, 1H), 4.60 (s, 1H), 3.79 (s, 3H), 2.15 (d, *J* = 10.2 Hz, 6H), 1.88 (s, 3H)

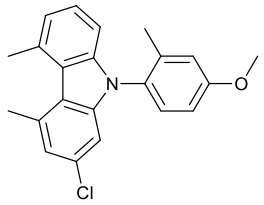
^{13}C NMR (151 MHz, $CDCl_3$) δ 157.44, 144.63, 141.08, 139.53, 137.87, 137.65, 136.26, 134.36, 132.00, 130.72, 129.97, 127.72, 119.47, 116.27, 112.32, 109.78, 102.56, 55.56, 21.33, 19.76, 18.41

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3401, 2922, 1581, 1503, 1465, 1289, 1221, 1049, 854, 772

HRMS (ESI): m/z = calcd for $[C_{22}H_{22}ClINO + H]^+$: 478.0429 found 478.0430

$[\alpha]_D^{20}$: -69.6 (c = 0.51, $CHCl_3$)

2-Chloro-9-(4-methoxy-2-methylphenyl)-4,5-dimethyl-9H-carbazole (11)



11

The reaction was performed following general E, with the following exceptions: No ^{1}H-qNMR-analysis of the crude product was performed. Hence no 1,3,5-trimethoxybenzene was added after the workup. The reaction was performed in DMF at 70 °C, using *t*-BuOK as base. Starting from 101.6 mg 4'-chloro-2'-iodo-N-(4-methoxy-2-methylphenyl)-6,6'-dimethyl-[1,1'-biphenyl]-2-amine (0.21 mmol, 1.0 equiv) 60 mg of the title compound (0.17 mmol, 81%) were obtained as a colourless solid after column chromatography on silica gel(petroleum ether / ethyl acetate: 98 / 2).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.24 (d, *J* = 7.7 Hz, 1H), 7.19 (d, *J* = 8.5 Hz, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 7.03 – 7.00 (m, 1H), 6.98 (d, *J* = 2.9 Hz, 1H), 6.93 (dd, *J* = 8.6, 2.9 Hz, 1H), 6.85 – 6.79 (m, 2H), 3.91 (s, 3H), 3.04 (d, *J* = 8.7 Hz, 6H), 1.86 (s, 3H)

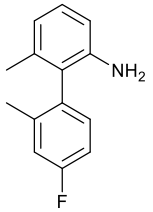
^{13}C NMR (151 MHz, $CDCl_3$) δ 160.01, 142.99, 142.63, 139.10, 133.77, 132.19, 131.07, 130.61, 128.30, 125.91, 123.45, 123.03, 122.10, 121.26, 116.70, 112.80, 108.03, 107.57, 55.66, 26.20, 25.96, 17.75

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2931, 1586, 1507, 1445, 1307, 1250, 1221, 1158, 892, 762

HRMS (ESI): m/z = calcd for $[C_{22}H_{20}ClNO + H]^+$: 350.1306 found 350.1307

$[\alpha]_D^{20}$: 17.2 (c = 0.49, $CHCl_3$)

4'-Fluoro-2',6-dimethyl-[1,1'-biphenyl]-2-amine (26)



26

The reaction was performed following general procedure A. 747 mg 2-bromo-3-methylaniline (4.01 mmol, 1.0 equiv) were reacted with 1.23 g of (4-fluoro-2-methylphenyl)boronic acid (7.96 mmol, 1.99 equiv). 812 mg of the title compound (3.77 mmol, 94%) were obtained as a beige solid after column chromatography (petroleum ether / ethyl acetate: 97/3).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.14 – 7.05 (m, 3H), 7.01 (td, *J* = 8.5, 2.7 Hz, 1H), 6.73 (d, *J* = 7.6 Hz, 1H), 6.65 (d, *J* = 8.0 Hz, 1H), 3.35 (s, 2H), 2.09 (s, 3H), 1.94 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 162.31 (d, *J* = 245.4 Hz), 144.00, 139.75 (d, *J* = 7.7 Hz), 137.15, 133.31 (d, *J* = 3.3 Hz), 131.48 (d, *J* = 8.2 Hz), 128.19, 125.98, 119.99, 117.24 (d, *J* = 21.0 Hz), 113.55 (d, *J* = 20.9 Hz), 112.69, 20.26, 19.51 (d, *J* = 1.7 Hz)

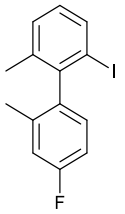
^{19}F NMR (282 MHz, $CDCl_3$) δ -115.56

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3466, 2969, 1738, 1580, 1534, 1458, 1366, 1217, 1099, 778, 526

mp 54 °C (from EtOAc)

HRMS (ESI): m/z = calcd for $[C_{14}H_{14}FN + H]^+$: 216.1183 found: 216.1184

4-Fluoro-2'-iodo-2,6'-dimethyl-1,1'-biphenyl (27)



27

The reaction was performed following general procedure B. Starting from 810 mg 4'-fluoro-2',6-dimethyl-[1,1'-biphenyl]-2-amine (3.76 mmol, 1.0 equiv) 818 mg of the title compound (2.51 mmol, 67%) were obtained as a colourless oil.

The reaction was repeated twice in scales of 0.40 mmol and 0.64 mmol with yields of 82% and 66% respectively.

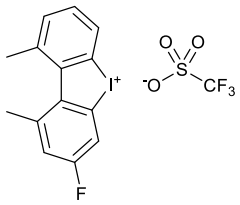
^{1}H NMR (600 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.9 Hz, 1H), 7.24 (d, *J* = 7.6 Hz, 1H), 7.03 – 6.92 (m, 4H), 2.01 (s, 3H), 1.98 (s, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 163.18, 161.56, 144.90, 139.03 (d, *J* = 274.3 Hz), 138.07, 136.66, 130.43 (d, *J* = 8.3 Hz), 129.93, 129.25, 116.93 (d, *J* = 21.0 Hz), 113.17 (d, *J* = 21.1 Hz), 101.53, 21.91, 19.79

^{19}F NMR (282 MHz, $CDCl_3$) δ -114.95 – -115.11 (m)

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3328, 2969, 1740, 1672, 1504, 1442, 1221, 1152, 816, 771, 580

3-fluoro-1,9-dimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (28)



28

The reaction was performed following general procedure C. Starting from 135 mg 4-fluoro-2'-iodo-2,6'-dimethyl-1,1'-biphenyl (0.41 mmol) 102 mg of the title compound (0.22 mmol, 53%) were obtained as a brownish solid.

The reaction was repeated once at a 0.31 mmol scale with 24% yield.

^{1}H NMR (300 MHz, MeOD) δ 7.96 (d, *J* = 8.0 Hz, 1H), 7.78 (dd, *J* = 6.9, 2.6 Hz, 1H), 7.71 (d, *J* = 7.6 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.52 (dd, *J* = 9.4, 2.6 Hz, 1H), 2.60 (s, 3H), 2.58 (s, 3H)

^{13}C NMR (75.5 MHz, MeOD) δ 161.89 (d, *J* = 255.6 Hz), 142.80 (d, *J* = 8.0 Hz), 140.94, 140.65, 138.70 (d, *J* = 3.4 Hz), 134.06, 129.67, 127.24, 120.88 (d, *J* = 21.9 Hz), 120.37 (q, *J* = 319.3 Hz), 119.24, 119.10, 114.99 (d, *J* = 27.6 Hz), 22.99 (d, *J* = 1.6 Hz), 22.83

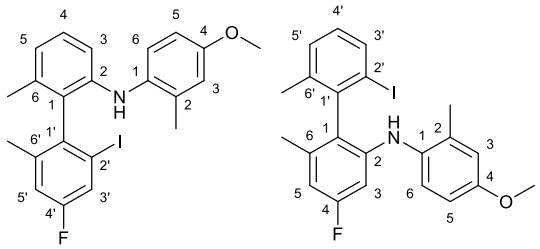
^{19}F NMR (282 MHz, $CDCl_3$) δ -78.02, -108.03

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 1739, 1595, 1442, 1366, 1282, 1230, 1160, 1025, 778, 637

mp 184 °C (from Et_2O)

HRMS (ESI): m/z = calcd for $[C_{14}H_{11}FI]^+$: 324.9884 found: 324.9887

4'-Fluoro-2'-iodo-N-(4-methoxy-2-methylphenyl)-6,6'-dimethyl-[1,1'-biphenyl]-2-amine (29a) & 4-fluoro-2'-iodo-N-(4-methoxy-2-methylphenyl)-6,6'-dimethyl-[1,1'-biphenyl]-2-amine (29b)



29a **29b**

The reaction was performed following general procedure D. 76.0 mg 3-fluoro-1,9-dimethyldibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.16 mmol, 1.0 equiv) were reacted with 26.1 mg *m*-cresidine (0.19 mmol, 1.2 equiv). 26.1 mg of title compound **29a** (0.06 mmol, 35%) and 16.5 mg of title compound **29b** (0.04 mmol, 22%) were obtained as faint yellow solids after column chromatography on silica gel (petroleum ether / ethyl acetate: 97/3).

29a:

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 7.9, 2.6 Hz, 1H), 7.16 – 7.05 (m, 3H), 6.80 – 6.66 (m, 3H), 6.45 (d, *J* = 8.2 Hz, 1H), 3.79 (s, 3H), 2.16 (s, 3H), 2.14 (s, 3H), 1.91 (s, 3H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 161.63 (d, *J* = 251.1 Hz), 156.88, 143.39, 140.88 (d, *J* = 7.8 Hz), 138.17 (d, *J* = 3.4 Hz), 136.56, 135.55, 132.97, 128.77, 128.69, 126.83, 124.39 (d, *J* = 23.3 Hz), 119.88, 117.75 (d, *J* = 20.8 Hz), 116.16, 112.12, 110.24, 101.94 (d, *J* = 8.5 Hz), 55.55, 21.70 (d, *J* = 1.7 Hz), 19.93, 18.42

^{19}F NMR (282 MHz, $CDCl_3$) δ -113.69

HRMS (ESI): m/z = calcd for $[C_{22}H_{21}FINO + H]^+$: 462.0725 found: 462.0728

$[\alpha]_D^{20}$: -81.7° (c = 0.47, $CHCl_3$)

29b:

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.86 (d, *J* = 7.9 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.08 (d, *J* = 8.5 Hz, 1H), 7.01 (t, *J* = 7.7 Hz, 1H), 6.79 – 6.67 (m, 2H), 6.41 (dd, *J* = 9.4, 2.5 Hz, 1H), 6.09 (dd, *J* = 11.5, 2.5 Hz, 1H), 4.62 (s, 1H), 3.79 (s, 3H), 4.19 (bs, 1H), 2.17 (s, 3H), 2.14 (s, 3H), 1.90 (s, 3H)

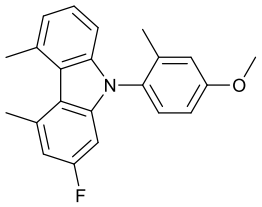
^{13}C NMR (75.5 MHz, $CDCl_3$) δ 163.58 (d, *J* = 241.2 Hz), 157.39, 145.11 (d, *J* = 11.5 Hz), 141.30, 139.81, 138.13 (d, *J* = 9.9 Hz), 137.61, 136.23, 132.13, 130.69, 129.89, 127.66, 125.14, 116.22, 112.26, 105.99 (d, *J* = 21.8 Hz), 103.21, 96.98 (d, *J* = 26.5 Hz), 55.56, 21.38, 19.99 (d, *J* = 2.0 Hz), 18.39

^{19}F NMR (282 MHz, $CDCl_3$) δ -113.75

HRMS (ESI): m/z = calcd for $[C_{22}H_{21}FINO + H]^+$: 462.0725 found: 462.0725

$[\alpha]_D^{20}$: -76.5° (c = 0.23, $CHCl_3$)

2-Fluoro-9-(4-methoxy-2-methylphenyl)-4,5-dimethyl-9H-carbazole (12)



12

The reaction was performed following general procedure E under the optimized conditions. Starting from 20.4 mg 4'-fluoro-2'-iodo-N-(4-methoxy-2-methylphenyl)-6,6'-dimethyl-[1,1'-biphenyl]-2-amine (44.2 µmol, 1.0 equiv), 12.3 mg of the title compound (36.9 µmol, 83%) were obtained as a colourless solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.25 – 7.16 (m, 2H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.98 (d, *J* = 2.8 Hz, 1H), 6.92 (dd, *J* = 8.6, 2.9 Hz, 1H), 6.82 (d, *J* = 8.1 Hz, 1H), 6.78 (dd, *J* = 10.3, 2.4 Hz, 1H), 6.49 (dd, *J* = 9.1, 2.6 Hz, 1H), 3.91 (s, 3H), 3.05 (d, *J* = 3.3 Hz, 6H), 1.87 (s, 3H)

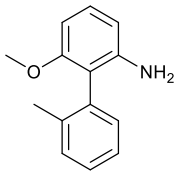
^{13}C NMR (151 MHz, $CDCl_3$) δ 161.42 (d, *J* = 242.1 Hz), 159.99, 143.29 (d, *J* = 12.2 Hz), 142.87 (d, *J* = 2.2 Hz), 139.09, 134.27 (d, *J* = 9.8 Hz), 131.79, 130.56, 128.48, 125.26, 123.41, 122.31, 119.03 (d, J = 1.6 Hz), 116.70, 112.79, 110.76 (d, *J* = 23.3 Hz), 107.87, 94.05 (d, *J* = 25.7 Hz), 55.66, 26.21, 26.11, 17.74

^{19}F NMR (282 MHz, $CDCl_3$) δ -117.14 (dd, *J* = 10.2, 9.1 Hz)

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2924, 1592, 1506, 1443, 1309, 1229, 1141, 1030, 995, 847, 776, 676

HRMS (ESI): m/z = calcd for $[C_{22}H_{21}FNO + H]^+$: 334.1602 found 334.1602

6-Methoxy-2'-methyl-[1,1'-biphenyl]-2-amine (30)



30

The reaction was performed following general procedure A. 1.01 g 2-bromo-3-methoxyaniline (4.95 mmol, 1.0 equiv) were reacted with 876 mg 2-methylphenylboronic acid (6.43 mmol, 1.3 equiv). 980 mg of the title compound (4.60 mmol, 93%) were obtained as a colourless solid.

The reaction was repeated in scales between 2.47 mmol to 4.95 mmol with yields ranging from 92% to 94%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.43 – 7.39 (m, 1H), 7.38 – 7.34 (m, 2H), 7.30 – 7.25 (m, 1H), 7.23 (t, *J* = 8.1 Hz, 1H), 6.54 (d, *J* = 8.1 Hz, 1H), 6.51 (d, *J* = 8.2 Hz, 1H), 3.78 (s, 3H), 3.61 (bs, 1H), 2.20 (s, 3H)

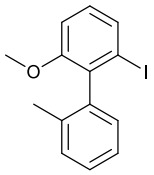
^{13}C NMR (151 MHz, $CDCl_3$) δ 157.71, 144.68, 138.08, 134.57, 130.61, 130.40, 128.83, 127.86, 126.34, 116.10, 108.66, 101.24, 55.74, 19.63

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3469, 3379, 3012, 2837, 1743, 1611, 1585, 1468, 1437, 1254, 1131, 1092

mp 67 °C (from pentane)

Elemental analysis: Found: C, 78.9; H, 6.8; N, 6.4. Calc. for $C_{14}H_{15}NO$: C, 78.8; H,7.1; N, 6.6%

2-Iodo-6-methoxy-2'-methyl-1,1'-biphenyl (31)



31

The reaction was performed following general procedure B. Starting from 1.07 g 6-methoxy-2'-methyl-[1,1'-biphenyl]-2-amine (5.05 mmol, 1.0 equiv) 1.53 g of the title compound (4.72 mmol, 93%) were obtained as an off white solid.

The reaction was repeated in scales between 2.26 mmol and 3.75 mmol with yields ranging from 73% to 80%.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.56 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.35 – 7.24 (m, 3H), 7.09 – 7.02 (m, 2H), 6.95 (dd, *J* = 8.4, 1.1 Hz, 1H), 3.71 (s, 3H), 2.03 (s, 3H)

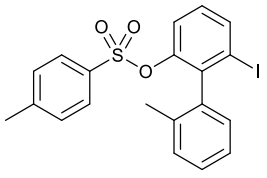
^{13}C NMR (151 MHz, $CDCl_3$) δ 157.13, 141.12, 136.30, 135.31, 131.01, 129.85, 129.74, 129.70, 127.95, 125.68, 110.56, 101.83, 55.93, 19.64

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3013, 2832, 1559, 1456, 1425, 1278, 1251, 1029, 1003, 821, 774, 758, 737

mp 91 °C (from pentane)

Elemental analysis: Found: C, 51.5; H, 4.1. Calc. for $C_{14}H_{13}IO$: C, 51.9; H,4.0%

6-Iodo-2'-methyl-[1,1'-biphenyl]-2-ol (32)



32

In a baked out 50 ml Schlenk flask containing a Teflon coated magnetic stir bar, 800 mg of 2-iodo-6-methoxy-2'-methyl-1,1'-biphenyl were dissolved in 10 ml anhydrous dichloromethane and cooled to -78 °C. 8.64 ml BBr_3 (8.64 mmol, 3.50 equiv) were added dropwise, the reaction stirred for 14 h and let warm to room temperature gradually. Ice cold

saturated, aqueous $NaHCO_3$ solution was added. The aqueous phases were extracted 3 times with dichloromethane. The combined organic phases were dried over $MgSO_4$, reduced *in vacuo* and used without further purification.

In an oven dried Schlenk flask, above crude product was dissolved in anhydrous dichloromethane and cooled to 0 °C. 473.5 mg *p*-toluenesulfonyl chloride (2.48 mmol, 1.1 equiv) and 27.5 mg 4-dimethylaminopyridine (0.23 mmol, 0.1 equiv) were added under N_2-counterstream. 938 µL triethylamine (6.77 mmol, 3.0 equiv) were added dropwise, the reaction allowed to warm to room temperature and stirred for 2 h. Water was added and the aqueous phase extracted with dichloromethane 3 times. The combined organic phases were dried over $MgSO_4$ and the solvent removed *in vacuo*. 954 mg of the title compound (2.05 mmol, 83%, 2 steps) were obtained after column chromatography on silica gel (petroleum ether / ethyl acetate: 90 / 10) as a colourless solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.52 (dd, *J* = 8.3, 1.1 Hz, 1H), 7.31 – 7.23 (m, 3H), 7.19 (d, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 8.1 Hz, 2H), 7.10 (q, *J* = 7.9 Hz, 2H), 6.73 (dd, *J* = 7.6, 1.4 Hz, 1H), 2.42 (s, 3H), 1.95 (s, 3H)

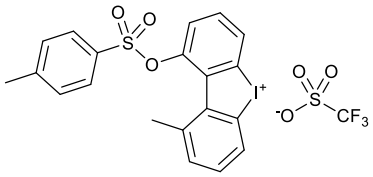
^{13}C NMR (151 MHz, $CDCl_3$) δ 146.45, 145.15, 140.14, 139.12, 137.72, 136.47, 133.09, 130.15, 129.96, 129.91, 129.71, 128.36, 128.14, 125.55, 122.69, 101.63, 21.81, 19.80

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3059, 1597, 1556, 1375, 1431, 1355, 1355, 1216, 1178, 1092, 881, 738, 553

mp 135 °C (from pentane)

Elemental analysis: Found: C, 51.8; H, 3.7; S, 7.0 Calc. for $C_{20}H_{17}IO_3S$: C, 51.7; H,3.7; S, 6.9%

1-Methyl-9-(tosyloxy)dibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (33)



33

The reaction was performed following general procedure C. 4.0 equiv of trifluoromethanesulfonic acid were used. Starting from 1.74 g of 6-iodo-2'-methyl-[1,1'-biphenyl]-2-ol (3.75 mmol, 1.0 equiv), 2.0 g of the title compound (0.33 mmol, 87%) were obtained as a colourless solid.

The reaction was repeated in scales between 0.28 mmol and 1.96 mmol with yields ranging from 75% to 96%.

^{1}H NMR (600 MHz, Acetone) δ 8.38 (dd, *J* = 7.9, 1.3 Hz, 1H), 8.04 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.92 (t, *J* = 8.0 Hz, 1H), 7.88 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.69 – 7.62 (m, 2H), 7.08 (d, *J* = 8.2 Hz, 2H), 6.99 (d, *J* = 8.0 Hz, 2H), 2.85 (s, 2H), 2.65 (s, 3H), 2.26 (s, 3H)

^{13}C NMR (151 MHz, DMSO) δ 146.81, 146.36, 140.74, 137.82, 136.21, 134.04, 131.40, 130.70, 129.92, 129.35, 128.53, 127.85, 127.04, 126.98, 120.74 (q, J_{C-F} = 323.7 Hz), 120.46, 120.14, 24.36, 21.05

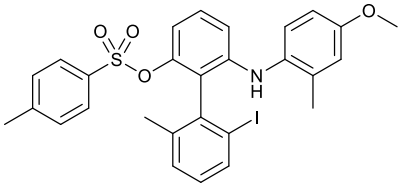
^{19}F NMR (282 MHz, Acetone) δ -78.96

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 1374, 1253, 1221, 1171, 1023, 869, 806, 735, 635, 557, 648, 513

mp 235 °C (decomposition)

HRMS (ESI): m/z = calcd for $[C_{20}H_{16}IO_3S]^+$: 462.9859 found 462.9856

2'-Iodo-6-((4-methoxy-2-methylphenyl)amino)-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (34)



34

The reaction was performed following general procedure D with an increased temperature of 60 °C and chloroform as the solvent. Starting from 200 mg of 1-methyl-9-(tosyloxy)dibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.33 mmol, 1.0 equiv), 58 mg of the title compound (0.097 mmol, 29 %) were obtained as a colourless solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.9 Hz, 1H), 7.46 (d, *J* = 8.0 Hz, 2H), 7.25 (d, *J* = 7.2 Hz, 1H), 7.18 (d, *J* = 7.9 Hz, 2H), 7.14 (t, *J* = 8.2 Hz, 1H), 7.08 (d, *J* = 8.5 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 6.80 (d, *J* = 8.2 Hz, 1H), 6.76 (d, *J* = 2.9 Hz, 1H), 6.71 (dd, *J* = 8.7, 2.9 Hz, 1H), 6.43 (d, *J* = 8.3 Hz, 1H), 4.76 (s, 1H), 3.78 (s, 3H), 2.41 (s, 3H), 2.20 (s, 3H), 2.13 (s, 3H)

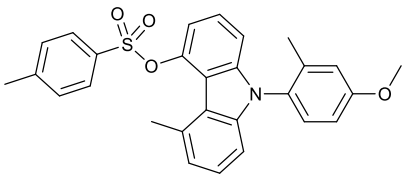
^{13}C NMR (75.5 MHz, $CDCl_3$) δ 157.50, 147.54, 145.42, 144.75, 140.78, 137.63, 137.25, 136.42, 134.19, 132.01, 130.39, 130.07, 129.67, 127.95, 127.77, 122.48, 116.21, 112.25, 110.84, 110.41, 102.75, 55.54, 21.80, 21.32, 18.40

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3385, 1608, 1496, 1456, 1346, 1204, 1172, 987, 827, 793, 687, 594

HRMS (ESI): m/z = calcd for $[C_{28}H_{26}INO_4S + H]^+$: 600.0700 found: 500.0710

$[\alpha]_D^{20}$: -37.8° (c = 0.58, $CHCl_3$)

9-(4-Methoxy-2-methylphenyl)-5-methyl-9H-carbazol-4-yl 4-methylbenzenesulfonate (13)



13

The reaction was performed following general E under the optimized conditions (see Table S1, entry 18). Starting from 29.9 mg 2'-iodo-6-((4-methoxy-2-methylphenyl)amino)-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (0.05 mmol, 1.0 equiv), 21.8 mg of the title compound (0.046 mmol, 92%) were obtained as a colourless solid after column chromatography (petroleum ether / ethyl acetate: 90 / 10).

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.74 (d, *J* = 7.7 Hz, 2H), 7.28 – 7.23 (m, 1H), 7.22 - 7.15 (m, 4H), 7.03 – 6.99 (m, 2H), 6.96 (d, *J* = 2.9 Hz, 1H), 6.91 (dd, *J* = 8.6, 3.0 Hz, 1H), 6.84 (d, *J* = 8.1 Hz, 1H), 6.77 (d, *J* = 8.1 Hz, 1H), 3.90 (s, 2H), 3.01 (s, 3H), 2.35 (s, 3H), 1.79 (s, 3H)

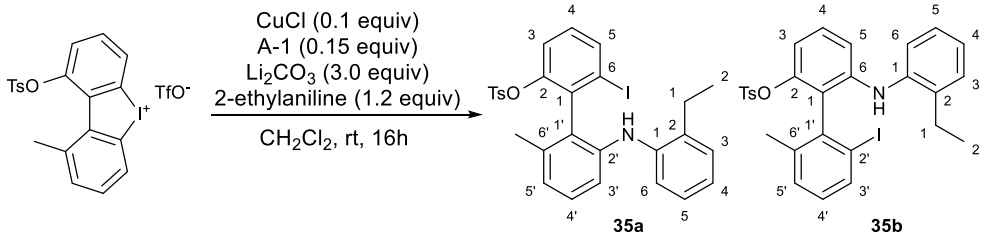
^{13}C NMR (151 MHz, $CDCl_3$) δ 159.99, 145.18, 144.46, 143.63, 142.15, 138.97, 134.43, 133.11, 130.51, 129.60, 128.79, 128.35, 126.60, 125.54, 122.89, 119.88, 116.65, 115.84, 112.70, 112.03, 108.26, 107.36, 55.65, 24.34, 21.74, 17.65

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2922, 1597, 1507, 1447, 1369, 1315, 1187, 1176, 1160, 1047, 861, 775, 748

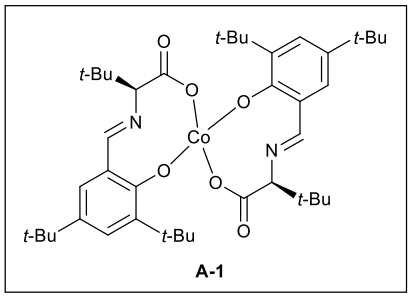
HRMS (ESI): m/z = calcd for $[C_{28}H_{25}NO_4S + H]^+$: 472.1577 found: 472.1579

$[\alpha]_D^{20}$: -10.2° (c = 0.58, $CHCl_3$)

2'-((2-Ethylphenyl)amino)-6-iodo-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate, 6-((2-ethylphenyl)amino)-2'-iodo-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (35a & 35b)



The reaction was performed based on the protocol developed by Zhang *et al.*[3] Chiral anion A-1 was synthesized according to literature. Starting from 29.7 mg 1-methyl-9-(tosyloxy)dibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.05 mmol, 1.0 equiv), 19 mg of title compound **35a** (0.033 mmol, 65%, 78%*ee*) and 5.8 mg of title compound **35b** of the title compound (0.01 mmol, 20%)



were obtained after column chromatography on silica gel (petroleum ether / ethyl acetate: 96 / 4).

35a:

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.94 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.54 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.37 – 7.29 (d, *J* = 8.3 Hz ,2H), 7.28 – 7.10 (m, 7H), 7.06 (td, *J* = 7.6, 1.7 Hz, 1H), 7.00 – 6.86 (m, 2H), 6.79 (d, *J* = 7.5 Hz, 1H), 5.11 (s, 1H), 2.46 (dq, *J* = 14.9, 7.4 Hz, 2H), 2.39 (s, 3H), 1.90 (s, 3H), 0.95 (t, *J* = 7.5 Hz, 3H)

^{13}C NMR (76 MHz, $CDCl_3$) δ 147.03, 145.28, 142.83, 140.69, 138.47, 137.77, 137.40, 135.29, 133.16, 130.62, 129.71, 129.10, 128.99, 128.69, 128.08, 126.59, 122.95, 122.24, 121.82, 120.21, 114.54, 103.20, 24.43, 21.80, 20.18, 14.23

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 3398, 1579, 1430, 1367, 1294, 1179, 1165, 1090, 883, 749, 664, 550

HRMS (ESI): m/z = calcd for $[C_{28}H_{26}INO_3S + H]^+$: 584.0751 found: 584.0756

35b:

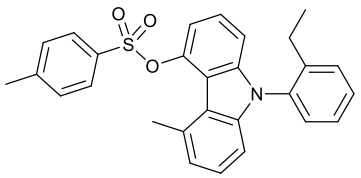
^{1}H NMR (300 MHz, $CDCl_3$) δ 7.76 (d, *J* = 7.9 Hz, 1H), 7.52 – 7.42 (m, 2H), 7.31 – 7.10 (m, 7H), 7.05 (td, *J* = 7.4, 1.4 Hz, 1H), 6.99 (t, *J* = 7.8 Hz, 1H), 6.88 (dd, *J* = 8.2, 1.0 Hz, 1H), 6.82 (dd, *J* = 8.3, 1.0 Hz, 1H), 4.95 (s, 1H), 2.44 (q, *J* = 7.5 Hz, 2H), 2.42 (s, 3H), 2.17 (s, 3H), 0.99 (t, *J* = 7.5 Hz, 3H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 147.61, 144.81, 144.17, 140.70, 139.01, 137.84, 137.57, 137.26, 134.14, 130.40, 130.13, 129.70, 129.64, 129.49, 127.96, 126.97, 124.59, 123.80, 123.31, 111.90, 111.78, 102.55, 24.73, 21.80, 21.32, 14.42

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 1580, 1521, 1455, 1349, 1208, 1176, 996, 856, 794, 743, 693, 564

HRMS (ESI): m/z = calcd for $[C_{28}H_{26}INO_3S + H]^+$: 584.0751 found: 584.0755

9-(2-Ethylphenyl)-5-methyl-9H-carbazol-4-yl 4-methylbenzenesulfonate (14)



14

The reaction was performed following general procedure E under the optimized conditions. Starting from 49.9 mg 2'-((2-ethylphenyl)amino)-6-iodo-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (0.086 mmol, 1.0 equiv), 35.7 mg of the title compound (0.078 mmol, 91%) were obtained after column chromatography on silica gel (petroleum ether / ethyl acetate: 96/4) as a yellowish solid.

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.69 – 7.64 (m, 2H), 7.46 – 7.38 (m, 2H), 7.31 (ddd, *J* = 7.7, 5.3, 3.8 Hz, 1H), 7.19 – 7.08 (m, 6H), 6.96 (dt, *J* = 7.2, 1.0 Hz, 1H), 6.94 (dd, *J* = 7.9, 0.9 Hz, 1H),

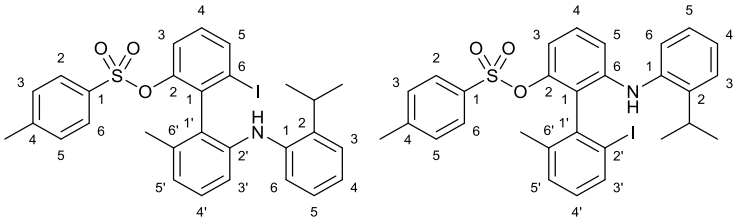
6.76 (dd, *J* = 8.2, 0.9 Hz, 1H), 6.68 (dt, *J* = 8.1, 0.9 Hz, 1H), 2.93 (s, 3H), 2.28 (s, 3H), 2.10 (q, *J* = 7.6 Hz, 2H), 0.83 (t, *J* = 7.6 Hz, 3H)

^{13}C NMR (151 MHz, $CDCl_3$) δ 145.20, 144.46, 143.77, 143.63, 142.29, 135.21, 134.43, 133.17, 129.97, 129.76, 129.62, 129.59, 128.78, 127.61, 126.62, 125.58, 122.98, 119.95, 115.91, 112.10, 108.37, 107.48, 24.36, 24.04, 21.75, 14.69

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2969, 1595, 1483, 1369, 1315, 1171, 1092, 878, 762, 550

HRMS (ESI): m/z = calcd for $[C_{28}H_{25}NO_3S + H]^+$: 456.1628 found: 456.1630

6-Iodo-2'-((2-isopropylphenyl)amino)-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (36a) & 2'-iodo-6-((2-isopropylphenyl)amino)-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (36b)



36a **36b**

The reaction was performed following general procedure D. Due to the steric demand of 2-isopropylaniline, an enantioselective ring opening reaction was not feasible. The reaction was instead performed with 0.5 equiv $[Cu(MeCN)_4]PF_6$ and no addition of PyBox ligand. Starting from 300.5 mg 1-methyl-9-(tosyloxy)dibenzo[b,d]iodol-5-ium trifluoromethanesulfonate (0.49 mmol, 1.0 equiv) 86 mg of title compound **36a** (0.14 mmol, 29%) and 55 mg of title compound **36b** (0.09 mmol, 19%) were obtained as off white solids. The enantiomers of racemic regioisomer **36a** were subsequently separated via preparative chiral HPLC.

36a:

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.95 (dd, *J* = 8.0, 1.1 Hz, 1H), 7.55 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.36 – 7.26 (m, 2H), 7.25 – 7.10 (m, 7H), 7.02 (dtd, *J* = 18.5, 7.3, 1.7 Hz, 2H), 6.84 (d, *J* = 8.2 Hz, 1H), 6.76 (dt, *J* = 7.4, 1.0 Hz, 1H), 4.81 (bs, 1H), 3.01 (hept, *J* = 6.8 Hz, 1H), 2.39 (s, 3H), 1.90 (s, 3H), 1.02 (d, *J* = 4.0 Hz, 3H), 1.00 (d, *J* = 4.0 Hz, 3H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 147.08, 145.26, 143.45, 140.90, 139.87, 138.47, 137.75, 137.34, 133.23, 130.68, 129.71, 129.01, 128.09, 126.42, 125.88, 123.13, 122.98, 121.85, 121.43, 113.85, 103.23, 27.45, 23.24, 22.66, 21.80, 20.19

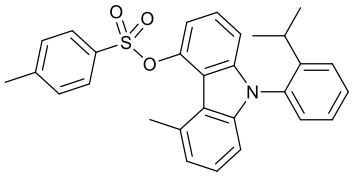
IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2923, 1582, 1465, 1356, 1215, 1178, 1091, 878, 740

HRMS (ESI): m/z = calcd for $[C_{29}H_{28}INO_3S + H]^+$: 598.0907 found: 598.0912

Enantiomer 1: $[\alpha]_D^{20}$: -58.0° (c = 0.66, $CHCl_3$)

Enantiomer 2: $[\alpha]_D^{20}$: 60.0° (c = 0.53, $CHCl_3$)

9-(2-Isopropylphenyl)-5-methyl-9H-carbazol-4-yl 4-methylbenzenesulfonate (14)



14

The reaction was performed following general procedure E under the optimized conditions. Starting from 34 mg enantiopure 6-iodo-2'-((2-isopropylphenyl)amino)-6'-methyl-[1,1'-biphenyl]-2-yl 4-methylbenzenesulfonate (0.06 mmol, 1.0 equiv, >99%*ee*), 24.3 mg of the title compound (0.052 mmol, 86%, 56%*ee*) were obtained after column chromatography on silica gel (petroleum ether / ethyl acetate: 95 / 5).

^{1}H NMR (300 MHz, $CDCl_3$) δ 7.80 – 7.70 (m, 2H), 7.61 – 7.48 (m, 2H), 7.37 (ddd, *J* = 7.8, 6.4, 2.5 Hz, 1H), 7.29 – 7.24 (m, 1H), 7.23 – 7.12 (m, 5H), 7.08 – 6.98 (m, 2H), 6.82 (dd, *J* = 8.1, 1.0 Hz, 1H), 6.75 (d, *J* = 8.1 Hz, 1H), 3.00 (s, 3H), 2.43 – 2.28 (m, 4H), 1.00 (t, *J* = 6.9 Hz, 6H)

^{13}C NMR (75.5 MHz, $CDCl_3$) δ 148.57, 145.21, 144.42, 144.15, 142.67, 134.38 (d, *J* = 1.5 Hz), 133.15, 129.87, 129.73, 129.62, 128.78, 127.48, 127.39, 126.62, 125.59, 122.94, 119.90, 115.87, 112.07, 108.35, 107.46, 28.02, 24.38, 24.11, 23.99, 21.78

IR (ATR, neat): $\tilde{\nu}$ [cm^{-1}] = 2968, 1597, 1482, 1456, 1371, 1315, 1177, 1091, 1049, 766

HRMS (ESI): m/z = calcd for $[C_{29}H_{27}NO_3S + H]^+$: 470.1784 found: 470.1785

$[\alpha]_D^{20}$: -12.7° (c = 0.45, $CHCl_3$)

3. Computational Details

3.1 Computation of Rotational Barriers

All calculations were performed in ORCA version 5.0.4[4, 5]. Geometries were optimized with Grimme's r²SCAN-3c composite DFT method[6], including DFT-D4 dispersion correction[7], gCP geometric counterpoise correction[8] and the triple-ζ basis set def2-mTZVPP. Vibrational analysis was performed to verify that each structure was a minimum or transition state on the potential energy surface (PES). Thermal and entropic corrections were obtained from unscaled vibrational frequencies for a standard state of 1 mol L^{-1} and 298.15 K, as implemented in ORCA.[9] Subsequently, electronic energies were calculated with the range-separated hybrid density functional ωB97M-V,[10] which utilizes VV10 dispersion correction[11] and the triple-ζ basis set def2-TZVPP.[12]

3.2 Computation of ECD-Spectra

Conformational sampling was performed for each structure using the Conformer Rotamer Ensemble Sampling Tool (CREST version 2.11.2).[13] Structural refinement and energetic sorting of the conformer ensemble was performed using the commandline energetic sorting tool (CENSO version 1.2.0) employing r²SCAN-3c.[14] Vibrational analysis was performed to verify that each structure was a minimum on the PES. Thermal and entropic corrections were obtained from unscaled vibrational frequencies for a standard state of 1 mol L^{-1} and 298.15 K, as implemented in ORCA.[9] Duplicate structures were manually removed from the ensemble. Electronic energies and Boltzmann-weights were calculated with the range-separated hybrid density functional ωB97M-V, quadruple-ζ basis set def2-QZVPP and C-PCM solvation model for acetonitrile.[10, 12, 15] For each conformer, ECD-spectra were obtained from TD-DFT calculations using the range separated hybrid functional CAM-B3LYP, quadruple-ζ basis set def2-QZVPP, C-PCM solvation model for acetonitrile[15] and employing the Tamm-Dancoff approximation (TDA).[15-17] The ECD-spectra of the conformers were summed based on their Boltzmann-weight to the final ECD-spectrum.

3.3 Mechanistic Investigations

Accurate electronic energies were calculated in ORCA 5.0.4, while all other DFT-calculations were carried out in Gaussian 16.[4, 5, 18] Conformational sampling was performed for each structure using the Conformer Rotamer Ensemble Sampling Tool (CREST version 2.11.2)[13] and each conformer ensemble restricted to 30 representative structures using the clustering algorithm. Based on two benchmarking studies for transition metal reactions by Iron and Janes[19] as well as Dohm *et al.*,[20] subsequent geometry optimizations were performed with the TPSS functional,[21] together with the D3(BJ) dispersion correction[22] and the def2-SVP basis set.[12] Vibrational analysis was performed to verify that each structure was a minimum or first order saddle point (transition states) on the PES. Intrinsic reaction coordinates were calculated to verify that each transition state connected the corresponding reactants and products on the PES. Thermal and entropic corrections were obtained from unscaled vibrational frequencies for a standard state of 1 mol L^{-1} and 298.15 K,

as implemented in ORCA.[9] Electronic energies were calculated with the range-separated hybrid density functional ωB97M-V,[10] the triple-ζ basis set def2-TZVPP[12] and the SMD solvation model for DMF.[23]

4. DFT-coordinates

4.1 Calculation of rotational barriers

Table S2: Energies and energy corrections for the calculation of rotational barriers of carbazoles at the ωB97M-V/def2-TZVPP//r²SCAN-3c level of theory.

Structure	Electronic energy [E_h]	Zero point energy [E_h]	Correction to	
			Enthalpy [E_h]	Gibbs free energy [E_h]
4	-905.741589	0.366508	0.386472	0.321325
TS[(*R*)-**4**–(*S*)-**4**]	-905.691898	0.366849	0.385565	0.323138
5	-1020.074876	0.385643	0.406642	0.339162
TS[(*R*)-**5**–(*S*)-**5**]	-1020.023551	0.385559	0.405468	0.340470
8	-1020.276730	0.397778	0.420974	0.348320
TS[(*R*)-**8**–(*S*)-**8**]	-1020.223798	0.398907	0.420472	0.352074

Coordinates of (*R*)-**4**

charge: 0, multiplicity: 1

44

C	4.09969248215780	-1.65361500032570	-0.38701923933684
C	2.61638770764461	-1.88249464117189	-0.27428952387296
C	2.16686073631741	-3.20062637227880	-0.36210927983407
C	0.81222727777060	-3.54109745868033	-0.39676088558352
C	-0.15641537477878	-2.55344749366876	-0.40205381975474
C	0.28427144712250	-1.23567598301519	-0.32265625960967
C	1.64602638686864	-0.85584756669972	-0.17652991683917
C	1.64119322159182	0.60071841730615	-0.03218556324066
C	0.28575728027940	1.01799646814795	-0.19818783826377
N	-0.51353741456071	-0.10548242521120	-0.37481252002641
C	-1.93242818312602	-0.18122371069728	-0.24852412525179

C	-2.70373616579727	-0.41319928967805	-1.38241910910130
C	-4.08638196979050	-0.51083205177152	-1.27425257202569
C	-4.68643430510817	-0.37809203164843	-0.02607386340983
C	-3.90561239966699	-0.16455070286229	1.10570373152520
C	-2.51498976685215	-0.07168190658180	1.02137769427241
C	-1.66405525802994	0.14583403211968	2.23886898162197
C	-0.12691154030226	2.35912490129749	-0.19991155082085
C	-1.53530870516888	2.81027752812665	-0.48043109384506
C	0.87005524761479	3.29039357084146	0.05584907806024
C	2.18484953841583	2.91006139088313	0.32604564854439
C	2.60288922356331	1.58332014019714	0.29980561355655
C	4.01652820918020	1.29165867710419	0.72425560014743
H	4.58609210187087	-2.56817391915238	-0.73613530034646
H	4.56354601670775	-1.37882636361071	0.56402268660166
H	4.32116697390719	-0.86250752507913	-1.10820703414689
H	2.90742987079884	-3.99257942704585	-0.43455891650056
H	0.52163542615352	-4.58566749376020	-0.45878017990638
H	-1.21401287383288	-2.78393543243894	-0.48033152726510
H	-2.20678896920871	-0.50561842463998	-2.34415477865811
H	-4.69027986393475	-0.68530971056546	-2.15954262193690
H	-5.76609467573130	-0.44839605561139	0.06941853810132
H	-4.38114846239375	-0.07427255438627	2.07921307300515
H	-1.20639814603062	1.14278539416727	2.23219443177324
H	-0.84105853843389	-0.57644866044032	2.27607722398070
H	-2.25789549813183	0.04656851605797	3.15064503163599
H	-2.23887042594128	2.52254433617800	0.30881691541095
H	-1.91969072428704	2.38621504759533	-1.41366170129453
H	-1.55867613616354	3.89985594068769	-0.56858283428883
H	0.60970203407415	4.34600617264186	0.06706931341111
H	2.90939605403278	3.67841564113644	0.58221350583881
H	4.04735635886107	0.49119789039138	1.46850846102174
H	4.45301956661340	2.18486552688597	1.17898237288686

H	4.66187223572477	0.99961260925582	-0.10836584623563

Coordinates of TS[(*R*)-**4**–(*S*)-**4**]

charge: 0, multiplicity: 1, imaginary frequency at 50.03 *i*cm^{-1}

44

C	3.92494241082992	-1.52281878915467	0.06541276379111
C	2.50490776351573	-1.73216154252226	-0.38178851066705
C	2.23899289382057	-2.85135591771884	-1.17499658414249
C	1.02377410997185	-3.02515586519277	-1.82945324617806
C	0.00267679819753	-2.10192877378231	-1.66109033630054
C	0.19658243265732	-1.06288476602622	-0.76655011136655
C	1.45624971696828	-0.81541613733091	-0.16053830641540
C	1.41271843862247	0.57499207222151	0.31741753565682
C	0.18665605164192	1.10203526538649	-0.15990054148196
N	-0.67871953191436	0.03881035181984	-0.56263868699277
C	-2.00428875624139	-0.04072599334803	0.00712772651252
C	-2.47996836532719	1.10887194200493	0.667943809444924
C	-3.77953113384452	1.23899316688667	1.12435485874756
C	-4.67472173778512	0.19344725596183	0.96182301581440
C	-4.18532720140967	-0.99108451681760	0.43990499718238
C	-2.86561757671982	-1.17403936424018	-0.00013746533030
C	-2.52021928176581	-2.61287582735966	-0.31016373474402
C	-0.01716590239644	2.46908128683077	-0.35170130974212
C	-1.12561720173421	3.03180067335996	-1.20180459067928
C	0.94432272346417	3.31244443955689	0.20806015915223
C	2.01956643776892	2.80664793122766	0.92796837616592
C	2.29527131012073	1.43795841980235	0.99403386589347
C	3.44144865901719	0.99270664358228	1.86626704511406
H	4.28653684152554	-0.53714760309357	-0.24094430265695
H	4.57364845856751	-2.27339180487051	-0.39299811401777
H	4.04500020519060	-1.60001798219935	1.14921956990982

H	3.043011804934 72	-3.559109975218 18	-1.357611140297 72
H	0.896010926082 88	-3.851640829906 98	-2.522174612856 62
H	-0.901330611874 09	-2.160332195249 51	-2.251031618762 52
H	-1.798919593765 54	1.921360443833 30	0.865746139747 04
H	-4.074930737826 87	2.159025059269 53	1.620570994203 77
H	-5.706819929171 54	0.271238523887 25	1.288216353998 94
H	-4.842956212869 63	-1.855970418062 52	0.399573896715 94
H	-1.532822358203 12	-2.898203647707 06	0.050246787949 08
H	-2.569481474291 40	-2.851906315276 14	-1.377323280083 23
H	-3.250285536719 38	-3.253831403003 26	0.190619069457 37
H	-1.653619212847 42	2.245198142091 22	-1.745188719859 44
H	-0.697507212975 22	3.727980009881 37	-1.931024514546 97
H	-1.867843588694 05	3.586168729983 89	-0.616278054132 53
H	0.834634824544 04	4.387602262188 04	0.086435663497 69
H	2.692698246386 74	3.496003638012 24	1.431885250853 22
H	4.399302895171 99	0.950293607513 38	1.338603575172 11
H	3.250880033494 15	0.012608731725 02	2.306808636886 35
H	3.557859173882 00	1.706731071054 10	2.687097689383 22

Coordinates of (*S*)-**5**

Charge: 0, multiplicity: 1

47

C	-4.151160328604 78	1.962573918572 22	0.690969358242 32
C	-2.834971295520 17	1.912227289925 78	-0.036343150028 38
C	-2.314311851686 02	3.112760601966 24	-0.508048894057 89
C	-1.052190280179 53	3.206354032087 42	-1.094571805334 59
C	-0.203120925227 43	2.112845357929 26	-1.194106736426 68
C	1.161879208828 39	2.266789744091 37	-1.809004521285 23
C	-0.717406207069 38	0.904303821342 18	-0.700350276462 47
C	-2.042686058449 87	0.750656399146 54	-0.190261809256 58
C	-2.197735635505 13	-0.665496021697 22	0.144392724947 19

C	-0.92939402411963	-1.26157291661081	-0.08974264963631
C	-0.62734050147027	-2.59198211327451	0.18454874253780
C	-1.65608119743656	-3.38390283221795	0.66161803711328
C	-2.94340389785231	-2.85935602702316	0.80298773278919
C	-3.25267727224058	-1.52541551420498	0.53561696082515
C	-4.70454605676974	-1.13210223715017	0.58901727433889
N	-0.06655486763444	-0.32386347605334	-0.63128913422234
C	1.32659386310855	-0.57705793599760	-0.77858234505652
C	1.78421281613413	-1.22997904638085	-1.89745315099181
C	3.15795920670043	-1.50536981563240	-2.04803709208014
C	4.05133673789716	-1.12352229031610	-1.07765252275041
C	3.60954363997211	-0.46604119019980	0.09541892650391
C	2.21449064301376	-0.19670027342245	0.26346972350610
C	1.77099384334737	0.44348933669532	1.44510352368453
C	2.67201279629080	0.81047994008695	2.41468629401087
C	4.05023427620913	0.55581282810019	2.24885127814254
C	4.50752953086049	-0.07025985213863	1.11587428187839
H	-4.97737323404747	1.54093616145283	0.11227727994864
H	-4.40520830842113	3.00226466306702	0.91387216644933
H	-4.09764324180822	1.42260572103424	1.64019397917042
H	-2.90761239165693	4.01642843564432	-0.39653083806053
H	-0.70748058778291	4.17020106415354	-1.46102031613907
H	1.25874932910561	3.26880637213758	-2.23556554159695
H	1.33530856049809	1.54018599155051	-2.60888944488198
H	1.96571357813253	2.13578354689815	-1.07616822309736
H	0.37024683246478	-2.98398619463006	0.01517835897802
H	-1.47305864142263	-4.42938642836532	0.89151754826577
H	-3.74868903682953	-3.52306347524932	1.10620730789558
H	-5.32635990158711	-2.03064338433208	0.61903388282257
H	-4.98892449033409	-0.55963028077683	-0.29772702783538
H	-4.95362571641834	-0.53242210565857	1.46859431404357
H	1.07333303215714	-1.51785592479064	-2.66670765137641

H	3.50516928231764	-2.01474153429267	-2.94188860581323
H	5.11284308307400	-1.32626857789643	-1.19557268878687
H	0.71140822092920	0.64219395016690	1.57418926479189
H	2.32198413986804	1.29993278156169	3.31873140799594
H	4.74879293414087	0.85479372985265	3.02488349701759
H	5.56773039502398	-0.27307623915105	0.98657055927768

Coordinates for TS[(*S*)-**5**–(*R*)-**5**]

charge: 0, multiplicity: 1, imaginary frequency at 31.03 *i*cm^{-1}

47

C	-4.35303794372540	0.56395184967031	-1.68689178513832
C	-3.04842919241750	1.22237055688507	-1.31611721819439
C	-2.71412265479610	2.40982575171005	-1.97104762919790
C	-1.49562081699121	3.05206147181334	-1.77723306215473
C	-0.47529894088840	2.46239212460319	-1.03271361235172
C	0.83775022066381	3.16223805277790	-0.83025231759976
C	-0.77873831226411	1.22423733727433	-0.46380289821889
C	-2.08578060288136	0.68368585866891	-0.43824172042123
C	-2.08124047011599	-0.30492838144376	0.65173711780312
C	-0.74174343891385	-0.37196835426677	1.12417613524467
C	-0.43964785199070	-0.86077636054040	2.38684305791549
C	-1.44527936963977	-1.48329864553510	3.11304333400272
C	-2.74243791442423	-1.52762886212739	2.61684185208469
C	-3.10306980079195	-0.89455267230019	1.42474998600147
C	-4.57183875156401	-0.77821616918254	1.12597441658618
N	0.11485722282989	0.40122836927415	0.28323609034240
C	1.31695148935198	-0.03321210958176	-0.38522100478865
C	1.49164647145830	0.37348815307284	-1.70105360215692
C	2.73130308518392	0.32004118671210	-2.35696936839921
C	3.83850305446686	-0.14999947554860	-1.70693531685111
C	3.68104882624661	-0.75745025327306	-0.44110711595739

C	2.39253606358409	-0.80586505400299	0.20208717256105
C	2.27211417955773	-1.71156440995058	1.28259323518135
C	3.35460059002856	-2.37852740798925	1.80851069070048
C	4.64139291647212	-2.18942761605473	1.27689807899828
C	4.78548911276852	-1.41351445294958	0.15587929438212
H	-4.27713322915950	-0.52396927878339	-1.64480822348711
H	-4.60594847322036	0.83738898722452	-2.71551307654300
H	-5.19245516546573	0.87246545105136	-1.05652089895830
H	-3.44597929769780	2.85515751731103	-2.64055399651575
H	-1.31971056084641	4.02259460800227	-2.23486275734011
H	0.67359965536278	4.24291665753516	-0.77866194635036
H	1.54190929731801	2.96717179761526	-1.64745702343316
H	1.32376168766798	2.83681685910036	0.09392647300380
H	0.53147968187119	-0.69158685331558	2.83202763840471
H	-1.22966021559516	-1.87762116390069	4.10156617737746
H	-3.52416366177372	-1.98196075914382	3.21936806549959
H	-5.15324740728449	-1.16888446530809	1.96474835361975
H	-4.86913737878417	-1.33180798853036	0.23177732782179
H	-4.85639645497623	0.26780938516281	0.98223492817454
H	0.65383091099656	0.79495594566150	-2.24062243643605
H	2.79837934615705	0.68854765375231	-3.37663458564951
H	4.82008491044337	-0.13699483892376	-2.17189633370366
H	1.29534427098417	-1.96066842463175	1.65902858179073
H	3.20135428762340	-3.07827306337087	2.62522750729880
H	5.49720501069692	-2.69746059015221	1.71148924342903
H	5.75348561447436	-1.32245792407170	-0.33055682837691

Coordinates of (*R*)-**8**

Charge: 0, multiplicity: 1

48

C	-4.05608451403879	-2.73169030089842	0.18082238553911

C	-2.59599787044891	-2.56456043044568	0.50281021088698
C	-1.89514839636112	-3.70932379284929	0.88633700449791
C	-0.51995912973797	-3.71451760000653	1.13434702650921
C	0.21931362037864	-2.55517820369994	0.98501560494840
C	-0.47221658016050	-1.40774434793318	0.61070306990214
C	-1.87893547975277	-1.34935345570571	0.38699492505977
C	-2.16703896782272	0.04158066203297	0.01791603741657
C	-3.30724546972171	0.83817483518545	-0.25073909647066
C	-4.73050036559270	0.36486180842937	-0.13159202518651
C	-3.11197295444012	2.17400361142911	-0.59534647909107
C	-1.85177663594522	2.78917465140600	-0.66769982436589
C	-1.74035438908611	4.23327330185165	-1.07334084585389
C	-0.72897826294909	2.04465826862846	-0.34673315762609
C	-0.90990802873626	0.70815745504946	-0.00227912247265
N	0.08570098634037	-0.16681775200805	0.37894018119897
C	1.47958700181346	0.11870983077813	0.37183429326717
C	2.09817130414365	0.57316944662293	1.53525080306260
C	3.45259560236378	0.85593467536733	1.54636772229688
C	4.19877615036650	0.68262143567136	0.37677477051803
O	5.52342350032567	0.98407146141612	0.47613118330159
C	6.33055450849011	0.82338954488159	-0.68617648335941
C	3.58052997563667	0.22768554796643	-0.79040816143317
C	2.21316601553032	-0.05987938831023	-0.80455171603803
C	1.53696885981373	-0.55029796215697	-2.05288985125460
H	-4.32754644425444	-3.78925392073678	0.23032687914340
H	-4.28261964322622	-2.37870615488092	-0.82909575298956
H	-4.70378474294774	-2.19193826608687	0.87607007488260
H	-2.44545932232485	-4.64191677538203	0.97587990459476
H	-0.02969767897209	-4.63834850919782	1.42700019525938
H	1.29306755006685	-2.52694593363064	1.14369095340554
H	-4.91969589798591	-0.07767392506487	0.85020672489473
H	-4.99003116260306	-0.37939109972295	-0.88850512605581

H	-5.413536019842 68	1.209558704692 11	-0.251851614088 47
H	-3.990683308999 59	2.781836474834 40	-0.800968599605 65
H	-1.983335032558 77	4.361775876948 12	-2.135089734903 90
H	-0.728677274859 68	4.615500778417 39	-0.912393780995 64
H	-2.437044054325 64	4.858835356727 87	-0.504736183973 60
H	0.266097485851 01	2.481642424750 10	-0.347761265220 74
H	1.500107180034 84	0.701502938249 60	2.432935371381 67
H	3.951398667780 26	1.210011404369 66	2.442475088173 53
H	7.339537487833 15	1.114478033510 95	-0.389714648749 28
H	5.989774215777 61	1.473531333837 78	-1.503126061188 84
H	6.338525948047 32	-0.220756569369 11	-1.026594035381 25
H	4.147931061746 69	0.088258567080 57	-1.703814580601 03
H	2.250358464785 48	-0.647372075804 22	-2.874756874243 93
H	0.741609613293 49	0.137796673214 76	-2.361618397050 00
H	1.064622427275 08	-1.524698639459 40	-1.884256991941 26

Coordinates of TS[(*R*)-**8**–(*S*)-**8**]

charge: 0, multiplicity: 1, imaginary frequency at: 53.05 *i*cm^{-1}

48

C	-3.865238537725 16	-2.515369472030 40	-1.089632879333 95
C	-2.619807739558 45	-2.420902304741 58	-0.244839090769 14
C	-2.113910720933 33	-3.601551040355 97	0.299373747015 76
C	-0.927320315685 43	-3.625603659806 45	1.029453717865 80
C	-0.121110127443 00	-2.498832077386 91	1.086927816276 90
C	-0.543182755511 15	-1.350757653076 44	0.427426833523 83
C	-1.875821406598 73	-1.236815170364 22	-0.047391302568 25
C	-2.151324745187 94	0.197261974996 32	-0.120131913681 25
C	-3.335858743396 83	0.964343311992 89	-0.157134902501 48
C	-4.715512291303 08	0.383724820450 53	-0.296556581663 39
C	-3.239460619437 52	2.335690267619 86	0.068182615180 08
C	-2.043782310104 86	2.966503019711 57	0.422362516236 37

C	-2.01992306275840	4.43812007405157	0.73261253109375
C	-0.88504387841298	2.20615801505526	0.51702929544660
C	-0.93237111446603	0.85098690009893	0.19747045395724
N	0.11125531177955	-0.09517110136315	0.34744547449749
C	1.45406834207727	0.17486481399025	-0.11679625252523
C	1.69352472156621	1.46513865680034	-0.63713007780065
C	2.94287106603382	1.94151315726232	-0.96973210209379
C	4.05185594079093	1.11635148266835	-0.81737394750622
O	5.27114772446766	1.66235203016886	-1.09996320457503
C	6.40827959133304	0.81597142987297	-0.98605070393530
C	3.82667750045005	-0.20518068349616	-0.46602434380611
C	2.55241353585184	-0.72120061774250	-0.16325581719130
C	2.53956172177529	-2.23028914749365	-0.06315570980308
H	-3.89828199202256	-3.50274023418403	-1.55977878574605
H	-3.86340277247134	-1.76980384252557	-1.88695398133760
H	-4.79041636185217	-2.40048710567227	-0.51675409477208
H	-2.68183838410245	-4.51942472429880	0.16914892031685
H	-0.61805058272600	-4.53425319493271	1.53727723762361
H	0.79255946694064	-2.50537005496941	1.66155064688143
H	-4.86279648721444	-0.43823009821251	0.40979472940291
H	-4.91655931673102	0.00061933090734	-1.30048257551203
H	-5.46439236868601	1.14951163893940	-0.07943213509062
H	-4.15214443893143	2.92737233757888	0.04688195409829
H	-1.95212002862256	5.02937422047015	-0.18916013743186
H	-1.15946208560109	4.69974826309735	1.35519068129082
H	-2.92999700776777	4.75073857085560	1.25393035131568
H	0.02144681703170	2.65841888728236	0.90249833410306
H	0.85872160223304	2.11895979302553	-0.83327338953616
H	3.06315550932537	2.94420758053345	-1.36717357580601
H	7.27258235672469	1.44268122648746	-1.21299625937525
H	6.36504756778779	-0.01441529195870	-1.70462640132016
H	6.50747816149269	0.41274467444828	0.03126951121673

H	4.64933704567912	-0.91157842653354	-0.46642700367303
H	3.39985169572499	-2.61708452676523	-0.61546232080298
H	1.64667166873897	-2.67412436543949	-0.50003714287320
H	2.63421284744695	-2.59634168501619	0.96468926568814

4.2 Calculation of ECD-spectra

Table S3: Energies and respective Boltzmann weights of the conformers of (*R*)-**7a** at the ωB97M-V/def2-QZVPP/C-PCM(acetonitrile)//r²SCAN-3c level of theory for the calculation of the ECD-spectrum.

# Conformer	Electronic energy [E_h]	Zero point energy [E_h]	Correction to Enthalpy [E_h]	Correction to Gibbs free energy [E_h]	Boltzmann weight [%]
1	-1318.624249	0.408063	0.435397	0.354566	27.6
2	-1318.624388	0.408063	0.435397	0.354566	19.05
3	-1318.623821	0.408027	0.435357	0.354425	15.33
4	-1318.623688	0.408005	0.435345	0.354391	12.35
5	-1318.623327	0.407799	0.435213	0.354341	7.38
6	-1318.623339	0.407764	0.435192	0.354270	6.72
7	-1318.623104	0.408059	0.435339	0.354632	6.08
8	-1318.622969	0.408005	0.435345	0.354391	5.47

Coordinates of (*R*)-**7a**, Conformer #1

charge: 0, multiplicity: 1

50

C	-0.00337085811436	2.93380252600906	2.17702962340225
C	-0.23906403042446	1.50063614074252	2.56406625851108
C	0.09770071506826	1.04091797881088	3.83286230785120
C	-0.09993896793921	-0.28864650239161	4.21453599481553
C	0.28843014170636	-0.75508972160893	5.59096681521763
C	-0.64666092710233	-1.17311194395806	3.28867434615777
C	-0.98667156821388	-0.71408133029410	2.01924391560070
I	-1.79435714045396	-2.11732884049172	0.64142979805318

C	-0.80961496841721	0.61192662727611	1.62681227285258
C	-1.18228545264374	1.10656279751079	0.27541314673898
C	-0.21859293582774	1.07938830368001	-0.75296333515251
N	1.05596142222648	0.59463673649043	-0.45990252203151
C	2.02956887271792	0.36856273794426	-1.46957570734467
C	2.76325582862284	1.44236313526693	-1.98994816905172
C	2.55047609991853	2.83827183647349	-1.47862779968146
C	3.72000100807094	1.19101627693273	-2.97867170264992
C	3.96708161872642	-0.10915403160853	-3.42114464833956
O	4.89031443768091	-0.43887364179209	-4.37186576330694
C	5.64497521110824	0.61742237184088	-4.95308162464392
C	3.24999656846163	-1.17775433878777	-2.87820039519632
C	2.28271638592941	-0.92970004816662	-1.92015933039860
C	-0.56186590231157	1.54574229497884	-2.02797866497357
C	-1.83427672492734	2.05001148574976	-2.25595569164383
C	-2.78258929383813	2.08776053451068	-1.23993995444081
C	-2.46572461576059	1.60836828892109	0.03253036258018
C	-3.49668915090869	1.60373955684421	1.12838879693410
H	-0.94186916456547	3.43253854768302	1.91022732566132
H	0.64241993322062	2.99295337083964	1.29398544937822
H	0.46623763056022	3.48779095083855	2.99385325118035
H	0.53032209028874	1.73807562158129	4.54811679993584
H	-0.13754609296529	-0.10322337050795	6.36094792580037
H	1.37742006046632	-0.73767889838971	5.71548256092936
H	-0.05501153210686	-1.77540221636776	5.77900786501767
H	-0.80666976210709	-2.21303402690331	3.55464701102578
H	1.07224133211893	-0.06866354648138	0.30324978473435
H	3.30217608660048	3.52199902177877	-1.88117792918181
H	2.60883691636642	2.85477619247497	-0.38493015732360
H	1.55811924311744	3.22133839341489	-1.74557638156893
H	4.28130132916096	2.02949843005076	-3.37620920883095
H	6.30631509327241	0.14582916634070	-5.68205251709922

H	6.24987154107909	1.14076560258854	-4.19987351320103
H	4.99530760137655	1.33985894153294	-5.46608226222522
H	3.45404110637806	-2.18395766875147	-3.22974006674631
H	1.69873561655043	-1.75128736131992	-1.51245650824549
H	0.161745380899O8	1.48721912495709	-2.83493259856041
H	-2.09206749286501	2.40814435827032	-3.24897838866381
H	-3.77744632223074	2.47853529551463	-1.43345617898178
H	-3.78327799806466	0.57692742108613	1.38724534828557
H	-4.39729904866776	2.13973727116856	0.81849298784641
H	-3.11625472773776	2.06510350081733	2.04662623667348

Coordinates of (*R*)-**7a,** Conformer #2

charge: 0, multiplicity: 1

50

C	-0.196877143443S6	3.07165587546296	2.06552478337691
C	-0.327058786880O6	1.64094189058137	2.50748348444911
C	0.03768572353426	1.25653831942672	3.79338236782098
C	-0.06107663248055	-0.06869216909767	4.22562191122069
C	0.34947244346175	-0.44977653422241	5.62176623212457
C	-0.53448905900722	-1.02669710267596	3.33328617591626
C	-0.90253059322111	-0.64308041486869	2.04661967087725
I	-1.59408555204896	-2.15542759212925	0.72173721904646
C	-0.82478412711657	0.67645334722107	1.60398027220539
C	-1.22675356983950	1.09004431281646	0.23385531744377
C	-0.25799844862966	1.09853491415303	-0.78994138934695
N	1.04810346209079	0.72400417482741	-0.47565905442143
C	2.03884092875020	0.53310652407881	-1.47648858786147
C	2.69883806577089	1.64641930485708	-2.03164418825385
C	2.384530181592S8	3.03758311742537	-1.56204936921762
C	3.668796897571S1	1.42676856233142	-3.00108200242353
C	4.01494844545879	0.13380411183744	-3.40582623736843

O	4.9912901999780 1	0.05983820503755	-4.35763959486009
C	5.37867038515678	-1.23586863937111	-4.79935317171623
C	3.37916042495034	-0.96777351763192	-2.83516817960344
C	2.38543540489886	-0.75025450672935	-1.88301315516750
C	-0.62813393280998	1.490470008374 36	-2.08243956025358
C	-1.93361047363503	1.888549811455 55	-2.33246340772768
C	-2.88793973529458	1.890964666449 02	-1.32133284324859
C	-2.54307884129298	1.483796167881 02	-0.03111294175227
C	-3.57669849004487	1.442116046783 69	1.06145837475485
H	0.22309073541475	3.690782376224 68	2.86235396522986
H	-1.16818526105431	3.487099338330 51	1.77459530352002
H	0.449896980864 50	3.145099101012 61	1.18424156818709
H	0.41385329719531	2.010910704309 67	4.48203856052165
H	-0.18119737472128	0.155144977750 91	6.36491302200927
H	1.42218676825207	-0.28289180241888	5.77242434468166
H	0.13966665682652	-1.50246380211382	5.82699069678068
H	-0.61611620390341	-2.06499312783896	3.63829120485906
H	1.11182602874902	0.09382662601157	0.31251988052901
H	3.06033645767292	3.765273931368 76	-2.01777516620762
H	2.48096882939401	3.100821200452 52	-0.47259407529935
H	1.35398124920963	3.323514505288 62	-1.80365141851733
H	4.19693303999113	2.263637616411 88	-3.44941337612211
H	6.15651862026438	-1.07628923915592	-5.54806596791347
H	4.53652911002657	-1.77137090141275	-5.25865163433666
H	5.78628289650126	-1.83574240213983	-3.97406676375248
H	3.62682622112491	-1.98228804966419	-3.12400649205568
H	1.85934956274616	-1.59851426286620	-1.45171872271034
H	0.10261789515165	1.459331606801 46	-2.88450085026587
H	-2.21184275135905	2.190661181342 34	-3.33849544175136
H	-3.90832268724953	2.198103597931 32	-1.53202868099552
H	-3.78417990466383	0.407310290723 01	1.36073410570468
H	-4.51441526257264	1.893817699170 12	0.72817553571583

H	-3.23826923093017	1.96800254000658	1.96132691137545

Coordinates of (*R*)-**7a,** Conformer #3

charge: 0, multiplicity: 1

50

C	0.04459463636941	2.89183420926571	2.28341505238065
C	-0.22634777297362	1.44828257450947	2.61129764331256
C	0.13404139379324	0.92358794795239	3.85011817006016
C	-0.10290294990814	-0.41130361504182	4.18323089808595
C	0.26602606384705	-0.94255358454714	5.54137067807336
C	-0.70846499883527	-1.23652033211631	3.23769142855270
C	-1.06752596787485	-0.71557093002390	1.99943725516817
I	-1.97827940644623	-2.02541663923624	0.59934051912469
C	-0.85114623122121	0.61873449596109	1.65471647488184
C	-1.22653063384357	1.18086002077156	0.33080002499485
C	-0.27025285175318	1.17794365887796	-0.70663768273593
N	0.96356056068060	0.58842654545938	-0.47966826103616
C	2.01420916773300	0.55342778521309	-1.42935300048526
C	1.93019607255864	-0.29559772286397	-2.55232605082796
C	0.74165573575357	-1.18825649867120	-2.75874873224905
C	2.98935615279136	-0.30937676675214	-3.45121399458262
C	4.13238132492624	0.46882266814355	-3.24702200598570
O	5.10084185348351	0.35012511973774	-4.20236345649658
C	6.28741184867578	1.11577718818628	-4.03144990996147
C	4.22697114634103	1.28383896053150	-2.11978524813599
C	3.15546009342029	1.32364167625086	-1.23072254005611
C	-0.59195162329808	1.76928869271396	-1.93645286714663
C	-1.84913467025417	2.32354844370697	-2.12515464432291
C	-2.79745643050242	2.31484665019955	-1.10772612131221
C	-2.48789205154575	1.75263513869433	0.13209690293299
C	-3.50521952021621	1.73312246075398	1.24064725938812

H	-0.88548053303323	3.42907308946430	2.06708397782702
H	0.66714568572769	2.98582845820880	1.38623131865014
H	0.55059438214649	3.39183375148293	3.11324607197975
H	0.61351423550154	1.57454067561832	4.57875214799035
H	1.21853110602355	-0.52625623865584	5.883323806588863
H	0.34904876021230	-2.03256620798996	5.534886813922229
H	-0.49509435733751	-0.67144350816517	6.28295521558978
H	-0.89681138227876	-2.28080282934931	3.46606735334774
H	1.21263140175245	0.44518845470315	0.48806288024192
H	-0.13574978516112	-0.62143424920218	-3.09297220081319
H	0.45434899332470	-1.67086723856579	-1.81902602642790
H	0.95841117238392	-1.95627226818733	-3.50529614109618
H	2.95742796755655	-0.95405552024442	-4.32515879207097
H	6.07230568177539	2.19315329821082	-4.02495993933287
H	6.92157400401792	0.87968963517123	-4.887724162945 86
H	6.81128461807148	0.84240267114488	-3.10515464463458
H	5.10181408571427	1.89367546737193	-1.92816061516362
H	3.20488752320855	1.97502157128229	-0.36170266343033
H	0.15225332680468	1.80471720994553	-2.72598265342069
H	-2.08799321589415	2.77988656058816	-3.08202351803057
H	-3.77897792951862	2.75090398520529	-1.26950702072746
H	-4.39864905450721	2.29628146155444	0.95959060729389
H	-3.10411059890577	2.15982270424394	2.16712700128944
H	-3.80843372288614	0.70488030668734	1.47285436615180

Coordinates of (*R*)-**7a,** Conformer #4

charge: 0, multiplicity: 1

50

C	-0.10561431443953	2.94662794400101	2.31003540600007
C	-0.31768946133316	1.49305928520529	2.63710320690178
C	0.03733787231802	0.98879421718537	3.885828397665 76

C	-0.14598555800629	-0.35464160981335	4.21847007322587
C	0.21584944409901	-0.86455172371459	5.58666934198115
C	-0.69081806495730	-1.20942788810045	3.26234281386927
C	-1.04421236514899	-0.70876410851836	2.01412187682506
I	-1.85938592635865	-2.06356571708495	0.59760544167757
C	-0.88153317622124	0.63309166391496	1.66944336347946
C	-1.25082857249920	1.17375009592871	0.33493212900053
C	-0.27044288353339	1.21362702035879	-0.67911871535265
N	0.98388581655880	0.68401918911976	-0.41939260409513
C	2.05734736437489	0.68328821089702	-1.34296129551020
C	2.03190389961206	-0.15765047488958	-2.46529971525324
C	0.87934627895834	-1.08672328361286	-2.71264906334024
C	3.11721751504550	-0.13608329552338	-3.34814450417708
C	4.22379681657803	0.67781747774526	-3.10671626894235
O	5.32450400342526	0.74518494775491	-3.91204306537975
C	5.33709025163938	-0.06594567544141	-5.08070052105560
C	4.25600720004859	1.48932983123053	-1.96992889107988
C	3.17294458315471	1.49380571494142	-1.10958784199854
C	-0.58947336972102	1.78722678984299	-1.91793443152332
C	-1.86612663233803	2.28195579730316	-2.13848871353661
C	-2.83773683410709	2.23002032471439	-1.14459652707563
C	-2.53248973281951	1.68513637262878	0.10400846227627
C	-3.57481016869683	1.61988753073294	1.18729627270604
H	0.36165187369470	3.47064739083200	3.14768660163103
H	-1.05471205933593	3.44103269675806	2.07491265106576
H	0.52893098152853	3.06664020627410	1.42450212629985
H	0.46972654053561	1.66288407576409	4.62282114959649
H	-0.56961365716401	-0.61886390219014	6.31151530112042
H	1.14481753815101	-0.41034847631120	5.94478731101634
H	0.34057489292494	-1.95058032958616	5.58816525608050
H	-0.83619736384694	-2.26065734923648	3.49016671860166
H	1.21529690167780	0.55521844837228	0.55479783227053

H	1.16442022545858	-1.88432365539000	-3.40380301980060
H	0.01789305148337	-0.55739021035997	-3.13834760284350
H	0.53310173323538	-1.53160778357950	-1.77444543925768
H	3.08692921096051	-0.79024851729540	-4.21274003691043
H	5.28809769926189	-1.13413433239983	-4.82864101100329
H	6.28502036249282	0.14371810358082	-5.57931439632867
H	4.50761495079494	0.18857839017667	-5.75466490314728
H	5.12559208748868	2.11317942298545	-1.79028798078798
H	3.17859236917416	2.14109074386984	-0.23616842804606
H	0.17199400395795	1.85763473670483	-2.68832652228112
H	-2.10243100795390	2.72627713884136	-3.10164568245196
H	-3.83431630256287	2.61940393223864	-1.33142460118041
H	-3.21502123075362	2.06070861884988	2.12400411796795
H	-3.83997189455213	0.57916262594513	1.41040712580827
H	-4.48410894898387	2.14543639844911	0.88507530629158

Coordinates of (*R*)-**7a,** Conformer #5

charge: 0, multiplicity: 1

50

C	0.38563749492102	2.57056308629766	2.48241239253080
C	-0.03075780909112	1.13667349107703	2.65696837342936
C	0.31488684538809	0.43036501436194	3.80466326045791
C	-0.03962843904579	-0.90912720310781	3.98393703407036
C	0.33169705236907	-1.63714755199609	5.24678934113272
C	-0.75214465189897	-1.55037636783606	2.97387065417705
C	-1.10203758542406	-0.84480583656035	1.82608180825896
I	-2.16662415465861	-1.88748733178021	0.31026559052823
C	-0.77104277327446	0.49713243296045	1.63832663100437
C	-1.13892273816633	1.25056940270044	0.41016847015750
C	-0.22352185529122	1.29322274324668	-0.66353674076906
N	0.97101659282010	0.60080267701816	-0.52572020771638

C	2.06164523242728	0.59077537883232	-1.41067885189531
C	2.67950321047829	-0.63741750301796	-1.72639330941549
C	2.14366427982188	-1.925004786664 26	-1.16539791465660
C	3.79088795658197	-0.63448100723153	-2.55832585656269
C	4.29082244902105	0.55089016207412	-3.10241703124111
O	5.37608346663156	0.41222000636861	-3.92324252748649
C	5.91738096387564	1.59617446727565	-4.49413915910199
C	3.68075203666120	1.76467949813835	-2.78908731458762
C	2.58264718339959	1.77292782125265	-1.93342621249545
C	-0.56680122621840	1.99622138423676	-1.82677590741109
C	-1.78411360845283	2.65655592806214	-1.89570154505499
C	-2.67882671350737	2.63102104386275	-0.83086088318161
C	-2.36513184834862	1.91934483893362	0.32793180621073
C	-3.33697752300162	1.85359094161469	1.47447304400244
H	0.91154691206502	2.93568026944983	3.36817990632811
H	-0.479748041706 65	3.21536069059500	2.29521242949475
H	1.04774865709019	2.67654820315934	1.61519285610793
H	0.88179646390966	0.93658327564548	4.58376296915667
H	-0.26684176316527	-1.27769921189077	6.09211227507956
H	1.38421464306046	-1.47398757087073	5.50048998073884
H	0.16453867949776	-2.71306599950195	5.15204674131049
H	-1.03256689915737	-2.59339527141101	3.08034438940309
H	0.97237778567427	-0.10328069270691	0.19671337092196
H	2.64173386247753	-2.78455911249698	-1.61989052417946
H	1.06516311920204	-2.01528355083437	-1.33977293249456
H	2.30005397046176	-1.99409461419219	-0.07980223533891
H	4.28383479997518	-1.56754290143749	-2.81666531126446
H	6.75842916860247	1.27428656326761	-5.11089869226242
H	6.27899063042030	2.28712138702079	-3.71987359832403
H	5.18012599124664	2.11106347958636	-5.12585463330031
H	4.05181968295656	2.70516327643561	-3.17914468251208
H	2.12996576760771	2.72048385269391	-1.65747823641513

H	0.10646477702496	1.99959952214814	-2.67650579613076
H	-2.04233602697765	3.19376482812678	-2.80432890050767
H	-3.62805843886436	3.15440425865053	-0.89962743093186
H	-4.18532912785177	2.52121998927526	1.30435144260470
H	-2.86304408575648	2.12912470884657	2.42342570319991
H	-3.72424499241038	0.83486246612134	1.59900901463111

Coordinates of (*R*)-**7a**, Conformer #6

charge: 0, multiplicity: 1

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C	0.25242894391211	2.70766281444012	2.43131345911165
C	-0.07890639966086	1.25605570096007	2.63801028697888
C	0.30040460847775	0.59899072601462	3.80444006620653
C	0.02421941365275	-0.75415517678410	4.01448270735753
C	0.42345949383330	-1.42813629643911	5.29865639686883
C	-0.64160814034106	-1.46086734691035	3.01600453076359
C	-1.02476185598684	-0.80487353786697	1.84987742645450
I	-2.01465927041880	-1.94501147057199	0.35337404069726
C	-0.77303265636589	0.54968432584949	1.63137583553399
C	-1.17854302962109	1.25113049665294	0.38452513446271
C	-0.26005286502246	1.32895216247832	-0.68416663976914
N	0.97822515016015	0.72230322965792	-0.52411374315508
C	2.05589303050334	0.75084212964121	-1.42674383550673
C	2.71194317649402	-0.44267081193797	-1.76117548235261
C	2.23353066426227	-1.75627803339829	-1.20776446978810
C	3.82239729973685	-0.39651789902855	-2.61013821320749
C	4.26368437551130	0.81278951502587	-3.14447852323828
O	5.32554014174311	0.94452617970215	-3.99585106072465
C	6.02320833305837	-0.23865967762219	-4.36189481746698
C	3.60574213837999	1.99867336087462	-2.80791059606390
C	2.52474688942141	1.96367083303588	-1.94709165013510

C	-0.63735002693028	1.98449308204452	-1.86426846821868
C	-1.89263970687056	2.56656492636877	-1.95456288967684
C	-2.79216235737697	2.50648296316684	-0.89523288624483
C	-2.44351536262321	1.84005226184811	0.28040561998977
C	-3.41801537712523	1.73817104543049	1.42209872124800
H	-0.649086927766627	3.29579421711544	2.22853466644581
H	0.90937575031793	2.83289210048812	1.56279262707398
H	0.75341686186261	3.12338874543859	3.30919089640181
H	0.83125234652668	1.15648287105080	4.57382428219362
H	1.43848895129228	-1.14424447564956	5.59418225930994
H	0.38332415970833	-2.51669969806777	5.20821710857204
H	-0.24802925105544	-1.13560588935313	6.11468794181199
H	-0.86006666580403	-2.51597479121384	3.14623366281152
H	1.02000710621281	0.02692076434143	0.20561072144678
H	2.42815275749093	-1.84148526780651	-0.12952605064695
H	2.74006261657613	-2.59333236125850	-1.69459701663017
H	1.15305013469193	-1.87585849671827	-1.34805980336935
H	4.31953299761213	-1.32855164076262	-2.85600003127553
H	6.46399408804641	-0.73315769742821	-3.48499651707175
H	6.82129826753198	0.08034697845054	-5.03469199966063
H	5.36680984663306	-0.94605517941472	-4.88755003095260
H	3.96892567704979	2.93674547309662	-3.21539811646421
H	2.03569833891672	2.88900898302526	-1.65749699302769
H	0.04199643939157	2.01436697879919	-2.70876933344390
H	-2.17652225291935	3.06865146547090	-2.87551791217997
H	-3.77177386246189	2.96770150027370	-0.98093634070943
H	-2.96919989625458	2.06318423568639	2.36761224876543
H	-3.74204776282782	0.70019562583190	1.56667337948876
H	-4.30504419887548	2.34766721247175	1.23224305608569

Coordinates of (*R*)-**7a,** Conformer #7

charge: 0, multiplicity: 1

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C	-0.34887549902340	2.93918870642299	2.52714024529818
C	-0.43614957509798	1.44949072648860	2.71991882957109
C	-0.01605718509805	0.86241949321168	3.91130801128379
C	-0.07243240931685	-0.51751058049553	4.11420501828862
C	0.35370419423495	-1.12205299230266	5.42402312671523
C	-0.55169538032649	-1.32408617504357	3.08329575700959
C	-0.97125085953671	-0.74113410756338	1.89290503855799
I	-1.66419719666727	-2.02156629431262	0.34814441564398
C	-0.93931368690112	0.63796847839384	1.68055750563367
C	-1.37930648554372	1.26249971293669	0.40485629943094
C	-0.43363583834228	1.45091451405255	-0.62440456220199
N	0.877972835171 86	1.05893328759726	-0.40042003628021
C	1.82984196225047	0.70572464094706	-1.37797584333185
C	3.19393666309522	0.92258701466182	-1.09412453549540
C	3.60732595001786	1.53998089981906	0.21193452401881
C	4.14365104499388	0.54673484346974	-2.03403432174466
C	3.77287496822481	-0.01987897992539	-3.25578666092199
O	4.80330916328799	-0.32478970372335	-4.10206746192436
C	4.46805386676958	-0.91571752270581	-5.35084505010400
C	2.42427325445142	-0.23751223649750	-3.53396811568078
C	1.46753137553648	0.11363687633631	-2.58560676507016
C	-0.83083234731682	2.08824891602880	-1.80917503789518
C	-2.14424181225919	2.50288948124707	-1.95988979191197
C	-3.08120197062936	2.30504020417219	-0.94945450401437
C	-2.70226607431916	1.69197205453236	0.24469781679805
C	-3.70682351985072	1.45588796151731	1.33945690039075
H	0.27414092394085	3.18846179295172	1.66059082770979
H	0.07442213056314	3.42264775262175	3.41123248889290
H	-1.33602719288221	3.37230221257844	2.33152624757807
H	0.36903528736565	1.49953950670115	4.70510112723910

H	0.64148675632098	-2.17012345746885	5.30535340178030
H	-0.46565804210028	-1.08377525453351	6.15208049921627
H	1.19982207996762	-0.57807843234793	5.85433519047218
H	-0.59405142555304	-2.40147943171969	3.20838005548925
H	1.06310343805589	0.72002557643607	0.53336174986935
H	3.41005638246699	0.86920698484965	1.05932825053594
H	3.05025698733731	2.46472495525740	0.40084361091303
H	4.67608177158649	1.76687367859264	0.21583304766860
H	5.20073325724444	0.70298530835449	-1.83782327678460
H	5.41448238242823	-1.07555845894934	-5.87057945544668
H	3.83154723204069	-0.25136665373360	-5.95184124331509
H	3.96084750756201	-1.88108112969627	-5.21550364333332
H	2.10170850960304	-0.69348337799353	-4.46263712025327
H	0.42020160014344	-0.09084685480045	-2.78459091046749
H	-0.10347743658361	2.26978644385387	-2.59311144960561
H	-2.43996811031137	2.99920963319475	-2.88021205975256
H	-4.10895980111455	2.62948999633957	-1.08439232332901
H	-3.36445869055018	1.85971088504243	2.29912470639999
H	-3.87169605323527	0.38203559475970	1.49043471229282
H	-4.66674419830167	1.91669034344398	1.09346932426628

Coordinates of (*R*)-**7a**, Conformer #8

charge: 0, multiplicity: 1

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C	-0.23289954320299	2.91819889901285	2.48858868830234
C	-0.36196794327934	1.43191031322728	2.68397077718549
C	0.06538746551987	0.83181879887023	3.86624168999289
C	-0.03002835082712	-0.54568370944821	4.07105163306170
C	0.40476480980059	-1.16370149475767	5.37174292958419
C	-0.55682942964952	-1.33659209823954	3.05129919614503
C	-0.98397221514757	-0.74060892153967	1.87002693174422

I	-1.75135634785949	-1.99795909993522	0.34179926537572
C	-0.91315733616742	0.63685680433254	1.65629734745550
C	-1.36232553217307	1.27589858603043	0.39103251575614
C	-0.43494178614790	1.43631335569621	-0.65937144541657
N	0.86784102541889	1.00093896324217	-0.46841080217802
C	1.78446034415072	0.63653147812637	-1.47628968933515
C	3.15269719635890	0.84145262108989	-1.24810314261173
C	3.62266206105152	1.46561285114570	0.03572316793945
C	4.07531404630890	0.44587241641458	-2.22134480437380
C	3.64780448831899	-0.12558245986163	-3.41872374271869
O	4.47838697772102	-0.52123225955570	-4.43050308996719
C	5.87477892969704	-0.33345869465104	-4.24390414519916
C	2.28343906082031	-0.33129299229714	-3.63824116668865
C	1.36749302717275	0.03454101495270	-2.66960397045173
C	-0.83869789851958	2.08729000052767	-1.83446779310241
C	-2.14179186937882	2.54247450879822	-1.95521312776123
C	-3.06114012684822	2.37285427379280	-0.92378694042979
C	-2.67446019453964	1.74660234065917	0.26110386979203
C	-3.66098528150516	1.54003652856187	1.37805044837181
H	0.22539315451852	3.38818412051271	3.36246713440598
H	-1.21045335085268	3.38157585495819	2.31540923322660
H	0.37719276357799	3.14794959222965	1.60758210925735
H	0.48726362906474	1.45644538068316	4.65123410876768
H	1.27376548620981	-0.64394049603210	5.78609036153893
H	0.66109592129614	-2.21916313697615	5.24646185109885
H	-0.39891677215259	-1.10406645466036	6.11567370760205
H	-0.63052889453701	-2.41212751999600	3.17794176708768
H	1.06442185659795	0.64452581901734	0.45641873988217
H	4.68814179324838	1.70455918242707	-0.01092532602223
H	3.47375485717120	0.79515009195879	0.89319872913857
H	3.06560375831589	2.38473197776672	0.24986236246718
H	5.12962644799423	0.60927838460979	-2.02636912215112

H	6.24484656629347	-0.90069342094084	-3.37836943704870
H	6.12423679385102	0.72923023403079	-4.11655286895440
H	6.35144422663401	-0.70908863159290	-5.15115705651854
H	1.96344963673074	-0.79754786677376	-4.56464965545779
H	0.31080873355427	-0.15907181302819	-2.82596180005261
H	-0.12450201289469	2.24576768191306	-2.63542013872853
H	-2.44289208776665	3.04806793496101	-2.86870084067343
H	-4.08107166637323	2.72937361002378	-1.03505827530112
H	-3.85844361812287	0.47168282947375	1.52901454315144
H	-4.61023375397035	2.03386790432064	1.15590421915276
H	-3.28317657328198	1.92790979211891	2.33096822505882

Table S4: Energies and respective Boltzmann weights of the conformers of (*R*)-**7b** at the ωB97M-V/def2-QZVPP/C-PCM(acetonitrile)//r^{2}SCAN-3c level of theory for the calculation of the ECD-spectrum.

# Conformer	Electronic energy [E_h]	Zero point Energy [E_h]	Correction to Enthalpy [E_h]	Correction to Gibbs free energy [E_h]	Boltzmann weight [%]
1	-1318.624290	0.408034	0.435376	0.354579	20.9
2	-1318.623708	0.408059	0.435394	0.354601	19.91
3	-1318.624080	0.408006	0.435337	0.354468	17.92
4	-1318.623624	0.407991	0.435330	0.354435	13.3
5	-1318.623091	0.407856	0.435223	0.354586	7.61
6	-1318.623111	0.407761	0.435194	0.354289	7.59
7	-1318.622849	0.408084	0.435343	0.354824	6.62
8	-1318.622745	0.408060	0.435340	0.354760	6.15

Coordinates of (*R*)-**7b,** Conformer #1

charge: 0, multiplicity: 1

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C	-3.31048250905254	2.11808159150659	0.68451705195073
C	-1.82728122714128	2.12917500044242	0.43218314269259

C	-1.20804667163837	3.25949552061010	-0.10189161508117
C	0.15923949250572	3.26793176434068	-0.37838852260275
C	0.81935283778959	4.49781440729933	-0.94164278796971
C	0.91587885712031	2.12987491122821	-0.11429984533399
C	0.32131106995081	0.99189233420820	0.44120813669845
N	1.05985946122906	-0.15083643361062	0.74893829496764
C	2.41785210352853	-0.30044690605740	0.35925449521050
C	2.74981687784103	-1.10064808286389	-0.72799835677702
C	4.07567233787898	-1.29701858292135	-1.10876778767402
C	5.08239834294005	-0.65051532128959	-0.39341244725115
O	6.41619712538639	-0.74578650883919	-0.67076610117918
C	6.79978265825576	-1.56296630337602	-1.77029447589922
C	4.75353984397160	0.15660134298487	0.70003074185242
C	3.43522202729464	0.33144576910756	1.10046357117052
C	3.10551045129071	1.14781546309965	2.31668637513292
C	-1.06173915155326	0.99202071315908	0.70791140885009
C	-1.68902291924767	-0.22080402159791	1.29476503881635
C	-2.22853041291767	-1.24083365317782	0.50744056293697
I	-2.13582463884094	-1.09163147629005	-1.61114064411220
C	-2.82370368830156	-2.37287712436488	1.05587243002207
C	-2.87528912851094	-2.49263018825208	2.43864953611237
C	-2.33244398824163	-1.50137601488418	3.24920984440588
C	-1.73505826854924	-0.36948143993307	2.69759258909221
C	-1.13706364614127	0.69322047791518	3.57619416276059
H	-3.81585256698136	1.42477738105131	0.00081416845256
H	-3.73917012852739	3.11258088567399	0.53769803134497
H	-3.54629211391899	1.78502303271803	1.70156348181258
H	-1.80604050814219	4.14186563922007	-0.31750068564449
H	0.11588259132851	5.09095666115477	-1.53315905808467
H	1.67075680073865	4.23652486144072	-1.57708273753593
H	1.19602013718360	5.14018631063284	-0.13590624858155
H	1.97355090716529	2.11194780613792	-0.36290628219874

H	0.51648649853130	-1.00331864566136	0.73133959222430
H	1.95210723326544	-1.57386479501820	-1.29550575062133
H	4.29717262823639	-1.93250277410672	-1.957940378663 54
H	7.88853791291794	-1.505798400099 86	-1.81976222407517
H	6.37330387180199	-1.193297421348 17	-2.71285822498417
H	6.49730350531702	-2.608136849865 55	-1.61788315970034
H	5.562088014568 68	0.629424766529 85	1.25047435334505
H	2.491505117420 65	0.563299873149 21	3.01058176755425
H	2.524646604596 65	2.041459335719 47	2.05901720180068
H	4.015318227076 50	1.464012386527 26	2.83263888691264
H	-3.236924524710 72	-3.143849043974 39	0.41508627350735
H	-3.338244760960 76	-3.369191408997 01	2.88270778054974
H	-2.369916861100 24	-1.608181322385 10	4.33020105596272
H	-0.078906167928 10	0.842384862811 64	3.33476978184047
H	-1.222310083619 65	0.421164223475 26	4.63139871563551
H	-1.630921833006 11	1.659332857470 16	3.42312563295515

Coordinates of (*R*)-**7b,** Conformer #2

charge: 0, multiplicity: 1

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C	-3.312203607249 76	2.282459140620 58	0.720046468889 12
C	-1.858186166831 47	2.255599401532 14	0.333799859381 54
C	-1.285253453095 03	3.332148290562 54	-0.342963934408 30
C	0.061099606400 54	3.315418226459 63	-0.710660512094 43
C	0.682674329433 48	4.509009952498 52	-1.385546912960 02
C	0.836774206751 25	2.200207549683 65	-0.412406565971 79
C	0.278044927856 91	1.096174001460 78	0.244098489883 69
N	1.024335927889 97	-0.038379026190 62	0.525830444979 20
C	2.401649060587 15	-0.177975676078 53	0.225176915436 58
C	3.339426859093 64	-0.186551300423 45	1.252586004207 40
C	4.697621535065 29	-0.364825261282 97	1.000116000468 58

C	5.12009082746520	-0.51079472531408	-0.32048174078144
O	6.41965488760801	-0.67653361473681	-0.70589949585331
C	7.40822642935748	-0.70180402331684	0.31660447635559
C	4.18262812522598	-0.50527990687607	-1.35732129205634
C	2.82387132106813	-0.35770856407581	-1.10839303980367
C	1.83041004478288	-0.42199715600922	-2.23130367488207
C	-1.07874191911357	1.13162984711684	0.62486757853662
C	-1.64841450396504	-0.01479319020921	1.37961508480395
C	-2.26537162879977	-1.09829676666493	0.74940108910234
I	-2.41694085482391	-1.13340974027200	-1.36687348867219
C	-2.79535884096456	-2.17045824215833	1.45948844229457
C	-2.69944815156198	-2.16556594079226	2.84548712577420
C	-2.08171946876931	-1.10687758766126	3.50156850867456
C	-1.55240441684010	-0.03149192676918	2.78844267751929
C	-0.88535543870444	1.11125123823764	3.50518768175506
H	-3.45383821160930	2.05089101197614	1.78190822092403
H	-3.87884989852052	1.53165947499482	0.15564855138804
H	-3.75176683478516	3.26252780952621	0.51867194208448
H	-1.89752207011791	4.19884080135879	-0.58082090305394
H	1.53259486892626	4.21740997235136	-2.00947939250694
H	1.05065140589919	5.22726139880975	-0.64244560722990
H	-0.04428141174084	5.03190201111927	-2.01415974715528
H	1.89170295125159	2.18664911986528	-0.67288893674994
H	0.64651943415339	-0.64843956465150	1.23581214408876
H	2.99946864146433	-0.04486270827350	2.27549959938750
H	5.39710013091911	-0.37226851359428	1.82754664442480
H	7.43206453569762	0.24398801681080	0.87517069019541
H	8.36256288444070	-0.84365266402910	-0.19351458740469
H	7.24216541883593	-1.53395392955582	1.01456022713200
H	4.54093199233254	-0.64851209228034	-2.37295624857563
H	2.29370846747213	-0.82152617373867	-3.13678780341899
H	1.41785100724484	0.56761668762841	-2.46240719847138

H	0.97791257929290	-1.05123017283330	-1.95574514695260
H	-3.27214753888868	-2.99363169009530	0.93899042666255
H	-3.10870367168413	-2.99628263916970	3.41316620297586
H	-2.00915255213093	-1.11239717071108	4.58607422465362
H	-0.86666109951563	0.93603148680428	4.58393632541721
H	-1.40642145799573	2.05591968245670	3.31397132189197
H	0.14353120389125	1.25386476279003	3.15558015401432

Coordinates of (*R*)-**7b,** Conformer #3

charge: 0, multiplicity: 1

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C	-3.24074620628421	2.21205381350857	0.86260405956739
C	-1.77253159499860	2.17769061025488	0.53562744772384
C	-1.13506712012010	3.30672096123890	0.02096021262799
C	0.21671134459780	3.27568563324914	-0.32251716412580
C	0.87753710015462	4.48142698205459	-0.93529297823376
C	0.94213059637957	2.10307307506115	-0.13385732040095
C	0.33000777648968	0.96438134047337	0.40094737932947
N	1.03977356794476	-0.21328875735538	0.63697048364985
C	2.37195610475446	-0.39835523318816	0.17897168751805
C	2.62049242676233	-1.17090763321502	-0.95852503481595
C	3.91184647462306	-1.39243644610992	-1.40394599367809
C	4.98217867657116	-0.81288190100135	-0.71884208934111
O	6.22116052587982	-1.06767514874538	-1.23355867403037
C	7.34208988426094	-0.49993872056628	-0.56705638121285
C	4.74369076390758	-0.03796866068938	0.41696640307009
C	3.44192924725324	0.16415651110735	0.88671664132199
C	3.20352325583091	0.94841649405210	2.14506627840673
C	-1.03925580875574	1.00272263480505	0.72914445631666
C	-1.68359933783279	-0.20684030419997	1.30417432220596
C	-2.29549862900817	-1.17876679894481	0.50895650454734

I	-2.29275336416838	-0.95872538929399	-1.60519667356298
C	-2.90700728863426	-2.30738203303850	1.046454938888464
C	-2.90089578573287	-2.47347155452977	2.42534474881438
C	-2.28590191773711	-1.53101574924006	3.24260461781471
C	-1.67228050329948	-0.40255393467036	2.70195947630121
C	-0.99676133647136	0.60707164286476	3.58696177311453
H	-3.63662953926416	3.22695220215558	0.77534173535189
H	-3.43983157877319	1.84762952113625	1.87673669898432
H	-3.80574251140985	1.56606088300079	0.17925057438635
H	-1.70642777370595	4.22050438177490	-0.12495223999114
H	1.94486295846881	4.51613704205383	-0.69746728122938
H	0.41451514500070	5.40884152774622	-0.58546093706572
H	0.78497675484029	4.45950895435897	-2.02811468680760
H	1.98789760408302	2.05931674995209	-0.42582528350813
H	0.46472179748117	-1.04479118592976	0.61685932722745
H	1.77850485049606	-1.59348189354708	-1.50146717133677
H	4.11210768505148	-1.99475291945156	-2.28416698393044
H	8.21864315331892	-0.81493111568670	-1.13592929506306
H	7.42643960237005	-0.87025301675308	0.46389510894848
H	7.29023882095575	0.59753238662477	-0.55782966768563
H	5.56482986588319	0.40323897192474	0.97124874870911
H	2.58462346902377	0.37119170587904	2.84057445081460
H	2.66317544136262	1.88148077802733	1.94449303161187
H	4.14737253060525	1.19603455475094	2.63745487762955
H	-3.37679829751645	-3.04040956688339	0.40013339718996
H	-3.37558235735179	-3.34802912525522	2.86088320511329
H	-2.27892362174514	-1.67409396214177	4.32003537451146
H	0.05456716937743	0.72625305196465	3.30284559610167
H	-1.04562932136589	0.30210403961592	4.63547037850621
H	-1.46017069955300	1.59507460080094	3.48809191971866

Coordinates of (*R*)-**7b,** Conformer #4

charge: 0, multiplicity: 1

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C	-3.35123375459397	2.26092191290739	0.63741804894425
C	-1.88115232012859	2.24623974146212	0.31700451828859
C	-1.28448967449236	3.33306092729100	-0.32156816593206
C	0.07803149456759	3.32889748582966	-0.62459122686256
C	0.70792936496583	4.50287947315206	-1.32518649377565
C	0.84893760203018	2.22085209154887	-0.28973711880312
C	0.26780815406217	1.10675700617098	0.32944228333307
N	1.01094352904642	-0.01938318299698	0.65057415558565
C	2.40061147655650	-0.15255286267715	0.41440955474899
C	3.28772588423015	-0.17972634102075	1.49533319067348
C	4.64728391033873	-0.34813391362736	1.30437268528769
C	5.14622357871313	-0.46846622771096	0.00502553066540
O	6.50023800225789	-0.61385076256910	-0.09690616414553
C	7.05278031817510	-0.74731285799943	-1.40087871522434
C	4.27050054540024	-0.44492329581922	-1.08019205898320
C	2.89119009600092	-0.30512635002509	-0.89080517647152
C	1.96286900263939	-0.34473286520198	-2.06947801067843
C	-1.10714073214170	1.12704859528962	0.63957090926834
C	-1.70157740929472	-0.02482157760234	1.36642209625542
C	-2.27959231309335	-1.11255360546129	0.70740211958924
I	-2.33353352680809	-1.14570707151090	-1.41393140895754
C	-2.83283793696738	-2.19013097836710	1.39091139257145
C	-2.80108920509359	-2.18640186426827	2.77987608102433
C	-2.22339176553048	-1.12344693427402	3.46487887837755
C	-1.67079152295232	-0.04254618610635	2.77817415948723
C	-1.04746067756503	1.10464074175387	3.52649937067092
H	-3.88426502492292	1.50082504342448	0.05317627500511
H	-3.79085426371692	3.23519564962065	0.40982766825560

H	-3.53880584917296	2.03474893179846	1.69336611917681
H	-1.89059588179157	4.19859666413138	-0.57863218324828
H	1.77350258328792	4.58229304534609	-1.09078636486691
H	0.22113889321049	5.44158211067100	-1.04410796347952
H	0.61628897699332	4.39919550898908	-2.41355194622467
H	1.91720769142271	2.22164105821955	-0.48840754224468
H	0.60419194221040	-0.63217844504292	1.34212473760023
H	2.89392505613916	-0.05993026352984	2.50157782907394
H	5.33832826828495	-0.37478007954119	2.14066464494784
H	8.13092314603280	-0.84181701622906	-1.25998731353997
H	6.84306790130327	0.13706088959055	-2.01817252735010
H	6.67306362197514	-1.64484948412415	-1.90806848082859
H	4.63869492773662	-0.56218489701485	-2.09364798460699
H	1.63533041676891	0.66158636326814	-2.35906724169726
H	1.05434386048703	-0.90523108952055	-1.82776562154596
H	2.44998211594996	-0.80620812387711	-2.93258038568094
H	-3.27813567824104	-3.01659329445160	0.848211158061318
H	-3.22901568502996	-3.02138320688338	3.327146008056 24
H	-2.20092674974313	-1.12988010121476	4.55155721072939
H	-1.56249562259928	2.04640260345674	3.30693324809442
H	-0.00243279886925	1.25227580295400	3.23092637538087
H	-1.08361557063840	0.93094618049193	4.60501152704256

Coordinates of (*R*)-**7b,** Conformer #5

charge: 0, multiplicity: 1

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C	-3.16929534676510	2.20236060649926	0.95726529444796
C	-1.73035478703900	2.21343116875953	0.51832510081005
C	-1.17739416845566	3.35028248032651	-0.06812820898676
C	0.14833274305456	3.35943101542597	-0.50718929563336
C	0.70946569777228	4.57250441241910	-1.19992290842170

C	0.93495309460571	2.22632037239463	-0.33462773120123
C	0.40870006379283	1.07838036268852	0.272428555860257
N	1.15144211446178	-0.07948260167104	0.45994097725511
C	2.52189917433513	-0.26499043857932	0.21286069354094
C	3.47128198273805	0.64128010067985	0.68143437313915
C	4.83163251655770	0.44447423040818	0.46102754351792
C	5.25336221483511	-0.70029952833055	-0.21390296572728
O	6.55764419850194	-1.00971396795431	-0.48556974496153
C	7.55106389110754	-0.09524447243907	-0.04108391936776
C	4.30824787687307	-1.62660678311725	-0.66072754828322
C	2.94824646060572	-1.42364046703478	-0.46916121891124
C	1.94441951270626	-2.42236058146094	-0.97384378986965
C	-0.93793511402797	1.07329369941110	0.68932057542612
C	-1.49261253378298	-0.14675005546790	1.33260864328390
C	-2.14144457330956	-1.14771905925411	0.60465902344469
I	-2.34453162177664	-0.95191468559553	-1.50172111702393
C	-2.66065679905503	-2.29065149916065	1.20541212750119
C	-2.52116654328019	-2.44193160393788	2.57901239991468
C	-1.86702775120599	-1.47019403332872	3.32873236368196
C	-1.34503735294114	-0.32745570242917	2.72506682753097
C	-0.61930145287178	0.70921899935604	3.53623040698405
H	-3.61430748532646	3.19574383040539	0.86023010186033
H	-3.27268580731415	1.87621488512395	1.99852905048473
H	-3.75692835273253	1.50451153189407	0.34821124109189
H	-1.79258406044145	4.23813693084490	-0.19481637221844
H	1.80239380931292	4.58499265758626	-1.16327778956236
H	0.33768334499912	5.49576983472941	-0.74461680674192
H	0.41261932997688	4.58708878040040	-2.25574584126762
H	1.95753576442323	2.22098110285532	-0.69775699168896
H	0.60523365460126	-0.91555718753424	0.60177402938811
H	3.14270266503305	1.51261004014533	1.23984500688636
H	5.53768090442593	1.17572378441113	0.83668883195650

H	7.42089685900522	0.89438010977160	-0.50092660895481
H	8.50795435870568	-0.51574748380799	-0.35554372274903
H	7.54220826948472	0.00775332588517	1.05296344196406
H	4.66153537067464	-2.51120453413198	-1.18323968033337
H	1.44670115442426	-2.95301505849009	-0.15021967261256
H	2.42673281027713	-3.17628243495313	-1.60028188928683
H	1.15858593673152	-1.93296641868828	-1.56093935837103
H	-3.16272919705537	-3.04586717940402	0.61097476161326
H	-2.92312196203580	-3.32726643192338	3.06325713269458
H	-1.75622064190827	-1.60091615362387	4.40201666286487
H	-1.07222536483220	1.69887711306058	3.41341601583897
H	0.42167152068697	0.79846367913263	3.20451936917731
H	-0.62506637855296	0.44856330770334	4.59764262727232

Coordinates of (*R*)-**7b,** Conformer #6

charge: 0, multiplicity: 1

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C	-3.27362450083870	2.14970897104022	0.86146841771103
C	-1.82096874494808	2.20336503355739	0.47363659975188
C	-1.28671456763152	3.34802647220717	-0.11482091510031
C	0.05326606296575	3.39662272407186	-0.50551338461742
C	0.59715280538708	4.61703517834702	-1.19904084765507
C	0.87165824971440	2.29508640609355	-0.28328812841944
C	0.36354663837593	1.14078802565600	0.32705865978185
N	1.14316046975869	0.01703310270148	0.56912667188421
C	2.52549045986369	-0.11436617998119	0.34656922853956
C	3.42694304901252	0.82567741259183	0.86170360085390
C	4.78907600126443	0.68276955891051	0.67510969818497
C	5.28248983603504	-0.43001114956551	-0.01111330462695
O	6.64225028905116	-0.49158907285380	-0.14128303548184
C	7.18509637374423	-1.60969718000090	-0.83116937921858

C	4.39573810000113	-1.38583147985356	-0.50363507421268
C	3.01473278030437	-1.23288826168095	-0.34333125832482
C	2.06782399935120	-2.26116299710433	-0.89726482079745
C	-0.99611932714434	1.09520228693502	0.69543499717810
C	-1.53040228684315	-0.13122579454445	1.34356818253856
C	-2.11928745685525	-1.16765815931713	0.61430723333569
I	-2.25664573770229	-1.01823159096357	-1.50132847428281
C	-2.61988762985170	-2.31643061695635	1.21961268632889
C	-2.52285033598899	-2.43700263113343	2.59989895794182
C	-1.92853416144275	-1.42925878774249	3.35183107043757
C	-1.42523819911836	-0.28053757146906	2.74364010984646
C	-0.76407676143170	0.79585515612398	3.55821532642533
H	-3.81565621927476	1.42369436512720	0.24310115014730
H	-3.74771752879009	3.12596010944089	0.733188082654 78
H	-3.40307123818613	1.83551635836449	1.90347358313575
H	-1.92746034525740	4.21094184915350	-0.28113288461222
H	1.68799102058481	4.66079939864463	-1.13579843383717
H	0.18863389431460	5.53445348106247	-0.76371846589509
H	0.32574091794905	4.61153460895226	-2.26174945460134
H	1.90709974445096	2.31984548458889	-0.60735273205423
H	0.62583990410361	-0.83942555201963	0.69770948768973
H	3.04512200326879	1.67170699446667	1.42541481702856
H	5.48966817993349	1.41136243297566	1.07041346016461
H	8.26753772458317	-1.46958468377009	-0.82335924386434
H	6.83216579583019	-1.65057105544774	-1.87104381306553
H	6.93781412690559	-2.55330593091867	-0.32501852556165
H	4.75699221903100	-2.25845424096430	-1.03684313064812
H	1.26518727852208	-1.79005311485084	-1.47626714583234
H	1.58778953729072	-2.84664285878765	-0.10074930097317
H	2.59290553928121	-2.96717659984885	-1.54539132721268
H	-3.07549151327043	-3.09949540057769	0.62377076706131
H	-2.91120847044452	-3.32635998610442	3.08787809145988

H	-1.85081366535218	-1.53581607593436	4.43068071577241
H	-0.80310333329425	0.55797165823157	4.62426872180967
H	-1.24194741350102	1.76783199677597	3.39567631872991
H	0.28583643628873	0.91044790637070	3.26463644450148

Coordinates of (*R*)-**7b**, Conformer #7

charge: 0, multiplicity: 1

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C	-3.52684459309721	2.12949831713834	0.65174122813141
C	-2.03043925001031	2.24558668876845	0.54853778717016
C	-1.43607519218831	3.45220779329906	0.18787059100188
C	-0.04738057612816	3.56513904297318	0.07437120825591
C	0.57646211955170	4.87657641133721	-0.32169928223825
C	0.74992495659468	2.45412193961438	0.31692476365567
C	0.17506027018493	1.22224854147287	0.66178175884500
N	0.94754471034114	0.10864430180065	0.95918427803448
C	2.23414641868235	-0.18083322802065	0.46167543055347
C	2.65310534367053	0.23801689455938	-0.79900152338086
C	3.92475625205148	-0.06712871306750	-1.27624990860619
C	4.78349229323308	-0.83302387999993	-0.48917613376563
O	6.05118405239849	-1.20081002681448	-0.84806481717741
C	6.51579650191101	-0.77851838613459	-2.12344873360269
C	4.35772066444235	-1.28035885398026	0.76373099359775
C	3.10075607789685	-0.95865746923675	1.25689141920830
C	2.66004420598555	-1.43915318130106	2.61066162767270
C	-1.22462777028204	1.12478951389122	0.78292639134692
C	-1.82724789481841	-0.16653973612725	1.20619633325087
C	-2.20211842455625	-1.15230591344326	0.28927926320476
I	-1.90383488393420	-0.82015759963710	-1.78535670369502
C	-2.76246595554301	-2.36235945854553	0.68491968215100
C	-2.94678822743700	-2.60018615982353	2.04134173476303

C	-2.56944587125239	-1.64507428057534	2.97867259389211
C	-2.00818029096212	-0.43176503232430	2.58114623532988
C	-1.58894134037188	0.59224583945328	3.60054809324245
H	-3.91706104108410	1.44882291092359	-0.11479012247423
H	-4.00432868815820	3.10323775155982	0.51738425406513
H	-3.83731464047466	1.72259567612769	1.62096229767311
H	-2.06355456854974	4.31948192125120	-0.00458110541115
H	1.63915520612400	4.90713736221066	-0.06576449870660
H	0.07840489545392	5.71721138051868	0.17175313457137
H	0.48988171314343	5.03618006859134	-1.40345152389207
H	1.83066032651824	2.54114149808477	0.26011155046217
H	0.42854541409712	-0.68247502890195	1.31363490555759
H	1.96961507149227	0.80159109141013	-1.42628651570303
H	4.21404658136190	0.27964142286108	-2.26137066321705
H	5.89565603978900	-1.18780794203024	-2.93303063473494
H	7.53170120970964	-1.16677694202068	-2.21623741235877
H	6.53775438152303	0.31752841339664	-2.20062601693200
H	5.04255894485464	-1.87929564372925	1.35753487241870
H	2.26795630069879	-0.61025250779210	3.21096545749051
H	3.48982356928528	-1.90170599276427	3.15032334787844
H	1.85871657758155	-2.18695831060457	2.53581060486827
H	-3.04661930023104	-3.10488287340207	-0.05248624283997
H	-3.38375018139868	-3.54051376125063	2.36493786186096
H	-2.71063713306776	-1.84297827720536	4.03803730188502
H	-0.52359506767109	0.83066286804970	3.50429779218624
H	-1.77518580696347	0.23032641479021	4.61490460877498
H	-2.12908937849693	1.53524006694912	3.46170499133560

Coordinates of (*R*)-**7b,** Conformer #8

charge: 0, multiplicity: 1

50

C	-3.53339080216999	2.12187658176855	0.75384923388008
C	-2.04478708537643	2.25073221719361	0.57796710044098
C	-1.47926348704323	3.46213653281115	0.18718262017900
C	-0.09901983686945	3.58714399151264	0.00632408966848
C	0.49394368607331	4.90138841311066	-0.42600989402841
C	0.71922393641785	2.48384020265176	0.21311361096784
C	0.17263557530035	1.24780706383774	0.58712221423629
N	0.96938765100290	0.14186614277784	0.84483481455245
C	2.24187418447022	-0.11847524610964	0.29532727098816
C	2.58120129137524	0.28571484123765	-1.00150939153482
C	3.82783291565942	0.00589846640516	-1.52930017464983
C	4.75740779850518	-0.71371593745290	-0.77422713021084
O	5.96150612404327	-0.94624246322845	-1.37937589601478
C	6.93334087361297	-1.67930600698021	-0.64582571659487
C	4.41872288458200	-1.14604859434089	0.50692254357393
C	3.16891399733452	-0.84450456639473	1.05654055734399
C	2.81653196373808	-1.30637605221604	2.44258001970762
C	-1.21887043706900	1.13776214932820	0.77518452456672
C	-1.78897244637940	-0.15804481627949	1.22860131972266
C	-2.20118221537337	-1.14769121983914	0.33206793469431
I	-2.00909544602632	-0.81539064836960	-1.75495664275202
C	-2.73203133262879	-2.36151116463381	0.75609468005471
C	-2.84740626557823	-2.59908555147922	2.12014289403042
C	-2.43155546555868	-1.63996006557119	3.03689729728168
C	-1.89984553300335	-0.42299796052220	2.61099243637508
C	-1.43925106319498	0.60579829701990	3.60741980636639
H	-4.02583293027816	3.09030612638132	0.63620734481866
H	-3.79311613482206	1.71920020950166	1.73967155787780
H	-3.95363816169434	1.43228894766825	0.01156718562634
H	-2.12312411784543	4.32331100924248	0.02392258190350
H	-0.01813203659508	5.74328141002040	0.05026680418424
H	0.39713082912610	5.03175568105325	-1.51085466218998

H	1.55781148913249	4.96015213165483	-0.17970931771850
H	1.79512190816930	2.58013085131129	0.10266118657276
H	0.47746078121891	-0.65910906379413	1.21517056779048
H	1.84698028448505	0.81364522768166	-1.60210475609003
H	4.09399417002157	0.31820777206822	-2.53411821821221
H	7.21496855932849	-1.15911133644261	0.28037355013009
H	7.80644818998730	-1.75405658017780	-1.29660902657274
H	6.57557854487978	-2.68939464387499	-0.40176679125991
H	5.12181240650952	-1.71137840401369	1.10888717991430
H	2.40708647508748	-0.48139330545249	3.03647005877879
H	3.69311305285813	-1.70747235902207	2.95759927994845
H	2.05448901976782	-2.09756733633470	2.42720555394308
H	-3.04681208557545	-3.10698870887693	0.03425860829840
H	-3.26101469662939	-3.54217457369652	2.46569191973919
H	-2.51923492973603	-1.83735465411115	4.10213856876600
H	-0.38130223319870	0.85082169978165	3.45978956042564
H	-1.57452943166665	0.24486413239730	4.63019491472607
H	-1.99146012237480	1.54502010839738	3.49260914945431

Table S5: Energies and respective Boltzmann weights of the conformers of (*S*)-**11** at the ωB97M-V/def2-QZVPP/C-PCM(acetonitrile)//r²SCAN-3c level of theory for the calculation of the ECD-spectrum.

# Conformer	Electronic energy [E_h]	Zero point energy [E_h]	Correction to Enthalpy [E_h]	Correction to Gibbs free energy [E_h]	Boltzmann weight [%]
1	-1401.352707	0.332999	0.35520507	0.285000	11.1
2	-1401.352677	0.333006	0.355197	0.285162	9.05
3	-1401.352699	0.332988	0.35518432	0.285214	8.78
4	-1401.352681	0.333021	0.35519114	0.285268	8.13
5	-1401.352656	0.332965	0.35517432	0.285303	7.62
6	-1401.352659	0.332982	0.35517699	0.285326	7.46
7	-1401.352687	0.333020	0.3552035	0.285363	7.4
8	-1401.352672	0.332996	0.35517976	0.285352	7.36
9	-1401.352665	0.333001	0.35516998	0.285404	6.92
10	-1401.352635	0.332996	0.35519415	0.285379	6.88
11	-1401.352620	0.333021	0.35519296	0.285385	6.73
12	-1401.352651	0.332978	0.3551461	0.285455	6.46
13	-1401.352525	0.332976	0.35513344	0.285379	6.12

Coordinates of (*S*)-**11,** Conformer #1

charge: 0, multiplicity: 1

42

C	-4.40371395618190	0.56407193836343	-0.24840897770972
C	-2.94747240001381	0.93505798747227	-0.18996836098485
C	-2.65031922150722	2.29615622917053	-0.26630038071450
C	-1.33605771220392	2.76290751602712	-0.29734401781509
Cl	-1.05474722541713	4.49358508246004	-0.38804259081022
C	-0.25705763872946	1.90471320618081	-0.28328139590552
C	-0.56061407873699	0.54880059151866	-0.20265264024713
C	-1.87781832673787	0.01102103707931	-0.11369377080414
C	-1.70880228359118	-1.44366612482464	-0.00884620036632
C	-0.30525857656522	-1.67685128468686	-0.08507847981968

C	0.29099558512146	-2.93191754919300	-0.02624393905761
C	-0.54929686525631	-4.01910216981052	0.12650287264474
C	-1.92928438689640	-3.83203138465649	0.23930133380202
C	-2.53578363110123	-2.57618349017050	0.18986482185065
C	-4.02295421150641	-2.52687864100862	0.40963046442235
N	0.36101851329566	-0.47300686625298	-0.20504369219590
C	1.77464490893154	-0.30844687738451	-0.18901287211142
C	2.48669569084142	-0.35430293026237	-1.38417599686560
C	3.86418026611981	-0.19729113892729	-1.39208565665653
C	4.52650493384333	0.01058885507101	-0.18353226852074
O	5.88184414845017	0.16294151091419	-0.23327312512999
C	3.81412778650048	0.05577764548790	1.01557374838449
C	2.42967577809409	-0.10476574805312	1.03214085750487
C	1.65305257596888	-0.06138730934097	2.31639801153953
H	-4.75048265755634	0.09583495179712	0.67533739177633
H	-4.60116742462346	-0.12891507720648	-1.07049386538345
H	-5.01003472720499	1.45743096158304	-0.41485797245322
H	-3.46116933526662	3.01415304587237	-0.32180487454104
H	0.76729731003440	2.25502192338649	-0.34267777516200
H	1.36935626401795	-3.03627047664996	-0.09499741082368
H	-0.13707329741657	-5.02250256200202	0.17608402214368
H	-2.56265602988502	-4.70159565583395	0.39045068706521
H	-4.27898782289855	-1.88012933204924	1.25332315558826
H	-4.39744502369299	-3.52816635161198	0.63616273395629
H	-4.56382549815986	-2.16354454767747	-0.46738479702632
H	1.94618864629293	-0.51478232058159	-2.31256466551878
H	4.43360048683848	-0.22969784859885	-2.31480790517827
H	4.34329206226162	0.21600114762146	1.95358928963570
H	1.04679794702762	-0.96602371275210	2.43591917825923
H	0.96100356346816	0.78860851216869	2.32682043717124
H	2.32030070100875	0.02731856745410	3.17678473582503
H	6.22055516303277	0.30404868990699	0.65827989023213

Coordinates of (*S*)-**11,** Conformer #2

charge: 0, multiplicity: 1

42

C	-4.39441245520883	0.54474468574454	-0.26183796730723
C	-2.93911167892240	0.91881560375601	-0.19628415256866
C	-2.64276035802299	2.28011062712774	-0.27230112690855
C	-1.32860850022723	2.74732848871402	-0.30195986159161
Cl	-1.04791208358313	4.47824783515566	-0.38872037356954
C	-0.24896200455619	1.88935090105777	-0.29269540957338
C	-0.55198838549667	0.53335006233233	-0.21532768444225
C	-1.86873315678516	-0.00370421488534	-0.11741546410237
C	-1.69988289561979	-1.45730826306163	-0.00540935387776
C	-0.29784052425628	-1.69247595190618	-0.09478396798179
C	0.29644283260125	-2.94851227163256	-0.03760255639627
C	-0.54397460821464	-4.03314436719421	0.13289535134958
C	-1.92179133177877	-3.84265542331616	0.26600330436583
C	-2.52608144241293	-2.58579975093310	0.21639267623687
C	-4.00809247378827	-2.52793636951763	0.46721983740244
N	0.36903394107907	-0.49001762658879	-0.22705186521786
C	1.78240729540152	-0.32498761492781	-0.18746407069820
C	2.50463194716958	-0.27273452238165	-1.37599109378848
C	3.88180985511071	-0.11142136504681	-1.35908061346970
C	4.53312887963781	-0.00255992167090	-0.13191087261538
O	5.88859844984974	0.15515971096420	-0.15686232761061
C	3.81011690639620	-0.05421320181998	1.06076861432812
C	2.42588464080302	-0.21513766565310	1.05198972849271
C	1.63587796819872	-0.26839481929550	2.32760891195732
H	-4.99809670004294	1.43161678083747	-0.46812251558231
H	-4.75456123918633	0.10993892051406	0.67341671178455
H	-4.58049958201609	-0.17710982491250	-1.06117470424172

H	-3.453946981113 02	2.997628498336 31	-0.329939525454 60
H	0.775054761195 22	2.240228268153 81	-0.353317539666 75
H	1.373797259857 05	-3.055015338451 07	-0.119299727719 47
H	-0.133052170606 68	-5.037074725064 57	0.182856022732 16
H	-2.554219852829 98	-4.709519480888 48	0.435705891086 72
H	-4.376860374292 99	-3.520001439579 67	0.739090951893 00
H	-4.568952323463 93	-2.196816236324 47	-0.410210856273 85
H	-4.244283415774 50	-1.849334434528 30	1.291338327562 12
H	1.972896569776 64	-0.360355087750 19	-2.319072868080 56
H	4.459207245839 42	-0.067491104761 61	-2.276331435749 35
H	4.330706531594 41	0.034534255247 43	2.013000117721 37
H	0.872477788843 58	0.517501683474 65	2.345738217313 40
H	2.283862914910 30	-0.142980322792 20	3.198004399216 54
H	1.108541198730 62	-1.224635688457 04	2.420124497924 88
H	6.218827551204 88	0.223010711925 50	0.746364373120 67

Coordinates of (*S*)-**11,** Conformer #3

charge: 0, multiplicity: 1

42

C	-4.396045531809 34	0.560437012661 02	-0.326992862221 92
C	-2.939841368890 15	0.931820911553 56	-0.270233484839 11
C	-2.639311715245 46	2.288948218908 37	-0.391983612572 90
C	-1.323809933589 28	2.751465903770 70	-0.430578050368 99
Cl	-1.038050953208 76	4.477635541860 41	-0.577049854094 50
C	-0.246469832589 91	1.892036296432 24	-0.383421954239 30
C	-0.553511912937 98	0.540093100287 68	-0.261108443289 62
C	-1.872473040200 88	0.009611950080 82	-0.155328387646 10
C	-1.708077416477 59	-1.440235436868 21	0.004414247169 06
C	-0.305659151496 76	-1.681007210881 96	-0.065363824307 99
C	0.285351013355 82	-2.935758910746 91	0.035774604881 87
C	-0.558721551544 99	-4.013160983886 78	0.231650553298 72

C	-1.93733278397613	-3.81602762425341	0.34489892153783
C	-2.53874480343462	-2.56028811745250	0.25109901033918
C	-4.02352324468686	-2.49368783056661	0.48182167734936
N	0.36467691351551	-0.48480007124735	-0.22932562320069
C	1.77882619190769	-0.32415146942429	-0.21136671427645
C	2.48335123620753	-0.31342559472698	-1.40873071759735
C	3.86368476818774	-0.15593635703141	-1.41097644913355
C	4.53077104586574	-0.00968825606646	-0.19566982224537
O	5.88399589509129	0.14924529263152	-0.11454342929079
C	3.82314502022375	-0.02011838104903	1.00661581975168
C	2.44105079758049	-0.17582522440885	1.01719353519194
C	1.66493216096477	-0.18294098468963	2.30233902427929
H	-4.75683807849684	0.14798771887159	0.61803104473530
H	-4.58481880736250	-0.17904716193201	-1.10955689737540
H	-4.99764262604553	1.44388186094274	-0.55308155420641
H	-3.44829203039959	3.00611977908015	-0.47780512082651
H	0.77882458504098	2.23855758911226	-0.44722539863922
H	1.36327375903716	-3.04655769041722	-0.03151959745343
H	-0.15027722157990	-5.01572593728933	0.31685485701856
H	-2.57346145377244	-4.67617248768839	0.53392625589855
H	-4.39867091225312	-3.47879173144063	0.76973281073052
H	-4.57182258388133	-2.18003890034178	-0.40981315515602
H	-4.26926406111776	-1.79726211401561	1.28819061705690
H	1.94035433163335	-0.42989408968575	-2.34214600947626
H	4.41377247004458	-0.14681290843408	-2.34910141347887
H	6.25877780994757	0.14685868668969	-1.00277587680191
H	4.37251769655225	0.09852530493773	1.93583338324036
H	0.91689214603587	0.61796630123666	2.30954440152940
H	2.32632275896857	-0.04820015599796	3.16086014149854
H	1.12043041483708	-1.12601583851398	2.42477734723158

Coordinates of (*S*)-**11,** Conformer #4

charge: 0, multiplicity: 1

42

C	-4.40073109513183	0.56732491184130	-0.30664355906669
C	-2.94594011499989	0.94079900216134	-0.23049250762243
C	-2.64641383755766	2.30032602279548	-0.32414619548115
C	-1.33110026601546	2.76446442036289	-0.34926541758662
Cl	-1.04654663227131	4.49358770118024	-0.45947648131742
C	-0.25298219559203	1.90517273605212	-0.31805378029215
C	-0.55928938155041	0.55078798939769	-0.22377984779598
C	-1.87801249867616	0.01782024071733	-0.12876100678782
C	-1.71334679792622	-1.43453839874575	0.00143498341781
C	-0.31123843722174	-1.67414114706419	-0.07674039042812
C	0.27905476201800	-2.93128742985540	-0.00458348934943
C	-0.56549072530317	-4.01195996396745	0.17091419845255
C	-1.94331859745999	-3.81620658222792	0.29579524032839
C	-2.54369938819697	-2.55812360247737	0.23180038539448
C	-4.02560674321282	-2.49221794268523	0.48056505983930
N	0.35896996740907	-0.47449642346044	-0.21436608845983
C	1.77324300841596	-0.31474795937295	-0.19923619992356
C	2.47247518263316	-0.27731837221716	-1.39909579316404
C	3.85293527005553	-0.12057536779624	-1.40370185674328
C	4.52528349324841	-0.00229657450341	-0.18829902961196
O	5.87897372468794	0.15422791621293	-0.10951601267052
C	3.82298166179238	-0.03958259195664	1.01659127466838
C	2.44087512145636	-0.19477884947713	1.02954275233788
C	1.67003238669992	-0.23156133132644	2.31734752685564
H	-4.76931251656303	0.13469277813000	0.62608872611158
H	-4.57944542229673	-0.15708474691305	-1.10582530075088
H	-5.00274103999704	1.45340672945249	-0.52098640937014
H	-3.45567760600708	3.01831560754353	-0.39982211240856
H	0.77211839997175	2.25353799520269	-0.37412624242539

H	1.35665768920383	-3.04167096954841	-0.07734973016783
H	-0.15763193029675	-5.01646932255184	0.23276871356532
H	-2.57900184629071	-4.67939904816487	0.47204381212479
H	-4.25858250028917	-1.80648203277309	1.29994610564236
H	-4.39921128371177	-3.48043102485652	0.75973089703233
H	-4.58484421156244	-2.16461874255771	-0.39914052563856
H	1.92548745623223	-0.37219530102428	-2.33262439083685
H	4.39901996162430	-0.09030767309688	-2.34370119481849
H	6.24982124756274	0.17178135682555	-0.99923230885170
H	4.37635817339369	0.05780043011145	1.94589463305289
H	1.13411981283788	-1.18144433521290	2.42456375427838
H	0.91514258229101	0.56245979262704	2.34202676812563
H	2.33364516659622	-0.10708989678079	3.17570104034166

Coordinates of (*S*)-**11,** Conformer #5

charge: 0, multiplicity: 1

42

C	-4.35890133200764	0.60015653026481	0.25845124974413
C	-2.92309171835126	0.94411489345993	-0.02715560011817
C	-2.62296004261394	2.29941037378019	-0.16741579081268
C	-1.31478894150194	2.74768365489728	-0.35156792755620
Cl	-1.02724392239205	4.47187575525027	-0.51958490678950
C	-0.24273391663022	1.88076234683256	-0.37982112851225
C	-0.55017687318887	0.53030232425771	-0.24339073254332
C	-1.86734270839711	0.00488797397390	-0.10146849257543
C	-1.70875632143364	-1.45047930040081	-0.00407220617329
C	-0.30489038594107	-1.69057579672204	-0.03923371908568
C	0.28292963194386	-2.94547579558386	0.07565240244442
C	-0.56869222575574	-4.02769415499182	0.20155712303361
C	-1.95315356726446	-3.84157210750265	0.17586302313033
C	-2.55169306413897	-2.58624226950256	0.06026923213996

C	-4.05151227709761	-2.550565824626 58	-0.05057174798136
N	0.36715883796512	-0.49540117741235	-0.20861044162266
C	1.78131050085790	-0.33545493255920	-0.188307184796 32
C	2.50269027050747	-0.46983735021942	-1.36821920355107
C	3.88377003797996	-0.32042196189682	-1.36949552196808
C	4.53442584687862	-0.03081856256178	-0.17105583696983
O	5.88730375892796	0.13256423381520	-0.08990971914661
C	3.81048130277614	0.10292077631112	1.01379934846362
C	2.42774003245647	-0.04900620036437	1.02413557039265
C	1.63761705909728	0.08648814352317	2.29353196676747
H	-4.44671037971666	0.00409950745998	1.17057965680920
H	-4.82144470534303	0.03672811049996	-0.55525072130508
H	-4.94061065422162	1.51377459197128	0.40136473201239
H	-3.42308993593523	3.02929078119751	-0.11159698634588
H	0.77983138157763	2.22265593390248	-0.49410856185346
H	1.36265781243349	-3.05554931467523	0.05499409239378
H	-0.16291196972902	-5.03057039167377	0.29534471074032
H	-2.59812620295504	-4.71419810495241	0.22868137831821
H	-4.37102549601894	-2.00208456272736	-0.94076358858636
H	-4.52762075096462	-2.08703186805596	0.81700106484835
H	-4.44016991112477	-3.56859923775789	-0.13317693631156
H	1.97173319842941	-0.69271716014205	-2.28911060542312
H	4.44680139781707	-0.42563117871492	-2.29392244221783
H	6.27466436502223	0.01896294958809	-0.96539179547522
H	4.34793971747146	0.32535663799966	1.93082827390246
H	2.29787563502463	0.21503595108395	3.15386954836118
H	1.01262304165975	-0.79795527223930	2.45957087001854
H	0.96128347389700	0.94773105521414	2.24364755420034

Coordinates of (*S*)-**11,** Conformer #6

charge: 0, multiplicity: 1

42

C	-4.37596936199630	0.54847638511401	-0.09167692287177
C	-2.91477674644359	0.89631319555621	-0.01127635395149
C	-2.60092773284542	2.25438749632895	0.04829837885811
C	-1.28090346520133	2.70612577223184	0.04827045947459
Cl	-0.97732986802367	4.43304970151647	0.13808428435850
C	-0.21327835380197	1.83838353756994	-0.04676461218660
C	-0.53381576593555	0.48568405411425	-0.10688578719041
C	-1.85613585526768	-0.04269855405519	-0.04484677728136
C	-1.70541551368373	-1.50212298718919	-0.08418157022061
C	-0.30797756160156	-1.74393983789858	-0.21825869950941
C	0.26969965989627	-3.00614078253217	-0.30155097844167
C	-0.58289235642655	-4.09228333611603	-0.23089175138026
C	-1.95612296277200	-3.90003310777638	-0.05772340173136
C	-2.54397048017905	-2.63756312406608	0.03102606917797
C	-4.02230913438242	-2.58879787331899	0.30461983870337
N	0.37311404111416	-0.54250643468035	-0.23726931724850
C	1.78873081299648	-0.39770939469667	-0.20643710069656
C	2.48347247003869	-0.15928608348662	-1.38884770758575
C	3.86187424298666	-0.00906998894274	-1.38069937329608
C	4.54315952751103	-0.10250644235204	-0.16844492515921
O	5.89910941156325	0.04955146587420	-0.20163783757636
C	3.84788408708570	-0.34009385816021	1.01806402048587
C	2.46209306982592	-0.48852512619182	1.01863602780674
C	1.70423222403860	-0.74067420244409	2.28997671107603
H	-4.72903298386291	0.02528600994011	0.80014541227189
H	-4.58222640321533	-0.08642058317431	-0.95695632829098
H	-4.97034482223163	1.45897244560993	-0.19776915156323
H	-3.40294234719913	2.98386246726645	0.07724202313966
H	0.81458108030058	2.18105141875318	-0.08341222842127
H	1.34411974626754	-3.11698917262528	-0.41205237919199
H	-0.18495399505980	-5.10084236757939	-0.29178826023256

H	-2.59778553035355	-4.77217633559796	0.03054532026671
H	-4.24239410345257	-1.99855082036362	1.19816088136078
H	-4.40036664194200	-3.59986144420126	0.47521378432256
H	-4.58871146962902	-2.16217857939548	-0.52685295743745
H	1.92858111408836	-0.09209859833397	-2.32021418974471
H	4.41758441718942	0.17824813148239	-2.29321007821880
H	4.39169426919942	-0.40623394341651	1.95915191215440
H	1.23774643227025	-1.73268797901423	2.27655985615437
H	0.89557214922252	-0.01213561429255	2.41464345158270
H	2.36350967048945	-0.68063166743063	3.15899011967808
H	6.25094502942275	-0.02993384202553	0.69244013855616

Coordinates of (*S*)-**11,** Conformer #7

charge: 0, multiplicity: 1

42

C	-4.35241218755379	0.57505369510101	-0.20819889579865
C	-2.88773237411481	0.90204199715628	-0.10913701835339
C	-2.55251864919624	2.25628748938784	-0.09028794274331
C	-1.22550697224682	2.68597116159546	-0.07856735391052
Cl	-0.89473094939711	4.40998389272193	-0.04410467689806
C	-0.17045041521309	1.79889245968234	-0.12037117848864
C	-0.51235244777068	0.45002714606901	-0.13913751546499
C	-1.84463080887299	-0.05419020473229	-0.08726172202621
C	-1.71780545267377	-1.51634717414669	-0.07382812863582
C	-0.32202602659983	-1.78505270509889	-0.16919358984623
C	0.23606644855540	-3.05852124135331	-0.19668887763554
C	-0.63593177567287	-4.12782358139540	-0.10860704226333
C	-2.00887406654349	-3.90742618725142	0.02776828933977
C	-2.57745226373978	-2.63340252524135	0.06162317412828
C	-4.05983214991539	-2.55187402671363	0.30244210713220
N	0.37931083678012	-0.59617313084341	-0.21418274405024

C	1.79618739301029	-0.47361304345222	-0.15719825711234
C	2.52323710534366	-0.31601133067346	-1.33372123199268
C	3.90368088206294	-0.19074357842828	-1.29964916665116
C	4.55404679609907	-0.22625039128526	-0.06765428508982
O	5.91305322005040	-0.10055221532005	-0.07513193592977
C	3.82641764522667	-0.38298978909072	1.11284645021377
C	2.43861557281281	-0.50706605612724	1.08729326675661
C	1.64546864814712	-0.67280603846465	2.35123923929328
H	-4.93043454406121	1.49048285213877	-0.35411750136323
H	-4.73100435044557	0.08491220551778	0.69176747648661
H	-4.55197925565348	-0.08354626085242	-1.05728016388188
H	-3.34269456794683	2.99895382982635	-0.10336191739932
H	0.86326256933066	2.12429866427298	-0.14840356425349
H	1.31059259843826	-3.19006314458303	-0.27961707851200
H	-0.25384761722254	-5.14412841304821	-0.12673553367643
H	-2.66719905489074	-4.76541382422261	0.13117416999846
H	-4.45814730908465	-3.54971117271546	0.50210480710037
H	-4.60238272012602	-2.14734815162533	-0.55565431873673
H	-4.28790502755477	-1.92554923010545	1.16896302189026
H	1.99187385853863	-0.29226484770520	-2.28076929438647
H	4.48458019832068	-0.06616833713080	-2.20721120237243
H	4.34624706793102	-0.40531760733366	2.06941316683345
H	0.86518574824725	0.09271259292482	2.42618350776467
H	2.28817860229705	-0.60096762289846	3.23162637949801
H	1.13891378130429	-1.64478584657864	2.36971073990422
H	6.24156201399991	-0.13516030797717	0.83058634113297

Coordinates of (*S*)-**11,** Conformer #8

charge: 0, multiplicity: 1

42

C	-4.35458122267112	0.56909802144543	-0.22635125108467

C	-2.89173009877708	0.90252971203753	-0.12206441997277
C	-2.56209328370034	2.25822453469392	-0.10863422387893
C	-1.23688635077440	2.69324048784839	-0.09249969761857
Cl	-0.91312034302790	4.418820887720 34	-0.06529888022112
C	-0.17807867777249	1.81026194849751	-0.12452580864237
C	-0.51441158182394	0.45995357519688	-0.13884351720247
C	-1.84490218705563	-0.04934293129255	-0.09058358707813
C	-1.71239370257351	-1.51088726830862	-0.07009527428253
C	-0.31527196525483	-1.77458016480140	-0.15927750105872
C	0.24760652811605	-3.04605715148824	-0.18075839454573
C	-0.62066181460690	-4.11830561927723	-0.09170850738854
C	-1.99484295588355	-3.90262903701895	0.03977475985451
C	-2.56825040072409	-2.63063100026062	0.06725225565831
C	-4.05144503299049	-2.55361644927877	0.30463067957987
N	0.38161766073208	-0.58317983196822	-0.20583228601389
C	1.79793328729258	-0.45461767462764	-0.15017284231396
C	2.51765643275225	-0.27401963046584	-1.32486989931716
C	3.90011503907610	-0.14097459553975	-1.28966330058357
C	4.55425376271218	-0.19359268707047	-0.05986256595480
O	5.90883004679106	-0.07287111250912	0.05815011233325
C	3.83162555888938	-0.37363894390179	1.11974643423609
C	2.44715763601376	-0.50380847561801	1.09349055392055
C	1.65737675889880	-0.69242967359443	2.35622341344730
H	-4.93536417472379	1.48127370052443	-0.38149553721774
H	-4.73587000267797	0.08380537072283	0.67511691454997
H	-4.54742707702127	-0.09610396807282	-1.07181107319786
H	-3.35517626648402	2.99761167240592	-0.12931101026178
H	0.85443589694043	2.13973067852489	-0.14713115966341
H	1.32299247270638	-3.17396506246716	-0.25826771706588
H	-0.23462678265427	-5.13319966549714	-0.10421580722573
H	-2.65016255739184	-4.76267441002894	0.14512239517982
H	-4.44601672870109	-3.55175391461293	0.51016562491309

H	-4.59407712431983	-2.15699191656976	-0.55712673597634
H	-4.28371454847263	-1.92254727915394	1.16655206976979
H	1.98443483080653	-0.23803458348571	-2.27041695650762
H	4.46160390221661	0.00123622918220	-2.21003642939276
H	4.37137836233637	-0.40519110306468	2.06160348575194
H	0.86545716206538	0.06033281136905	2.43843275878650
H	2.30098469552083	-0.61863581508229	3.23544986593401
H	1.16546753863670	-1.67209547907108	2.36667065368254
H	6.29485730758095	0.05358581395781	-0.81615759393095

Coordinates of (*S*)-**11,** Conformer #9

charge: 0, multiplicity: 1

42

C	-4.30777500240162	0.50510194106515	0.47459429517694
C	-2.86974052088806	0.85291440779570	0.20457110287886
C	-2.54116244975673	2.20869869542178	0.23117510543066
C	-1.22656272762154	2.65054685366777	0.07937214292540
Cl	-0.90247420140439	4.37551003450311	0.12756362106193
C	-0.17535672319605	1.77226026788442	-0.08138043032082
C	-0.51119898564806	0.42241157927369	-0.11418532726229
C	-1.83720887059505	-0.09035921296936	-0.01093148521164
C	-1.70953041721463	-1.54968094573003	-0.09896592841785
C	-0.31236725197198	-1.81123042732840	-0.19655818659206
C	0.24948216757006	-3.08173003926083	-0.25703572337635
C	-0.62311460837439	-4.15450115886780	-0.24857531783395
C	-2.00340073763094	-3.93934957789452	-0.21634315762571
C	-2.57615189255306	-2.66794902531647	-0.15861057623245
C	-4.07684757689326	-2.58903123081508	-0.22741300661748
N	0.38269060068699	-0.61803044974910	-0.22935857975968
C	1.80026796101699	-0.48999753429090	-0.22851156114526
C	2.48171964120862	-0.40074786643368	-1.43611117218214

C	3.86522631406259	-0.27656710936399	-1.45537521420662
C	4.55938564312257	-0.24375808418236	-0.24668107496553
O	5.91743500881882	-0.12432828773285	-0.18170734792546
C	3.87505278392428	-0.33438570439392	0.96562549505722
C	2.48978546416942	-0.45792648055575	0.99341059871483
C	1.74050403667080	-0.55172438365090	2.29115345313903
H	-4.39211853762583	-0.20251519861352	1.30339520668548
H	-4.80071067871654	0.06399461993378	-0.39494237551482
H	-4.86377704668365	1.40491427522173	0.74820415540049
H	-3.32349417460604	2.94154445689804	0.39583541028914
H	0.85275124698212	2.10497834234427	-0.17010428884381
H	1.32587108274889	-3.20876025292844	-0.31952478359686
H	-0.23804911431375	-5.16888123723474	-0.29284875360868
H	-2.66649491067135	-4.79891630959666	-0.25839402455238
H	-4.40199497054050	-1.92061077770765	-1.02912373871130
H	-4.52370282667300	-2.23597208604446	0.70551441927597
H	-4.48972818797084	-3.57948626055454	-0.43446714453393
H	1.91768937087352	-0.42963587608965	-2.36387205510164
H	4.39704655067955	-0.20570446549391	-2.40137985169843
H	4.44550023553769	-0.30534033067138	1.88930338349983
H	2.42779577288467	-0.55646099972447	3.13998982069496
H	1.13339959827990	-1.46319900591359	2.32789975964526
H	1.05299042167334	0.29413424120126	2.40708350943638
H	6.27504851304039	-0.06465939610177	-1.07501037347523

Coordinates of (*S*)-**11,** Conformer #10

charge: 0, multiplicity: 1

42

C	-4.36483629041580	0.58057585282068	0.26789968448747
C	-2.93186006439700	0.93802291597489	-0.01511591150105
C	-2.64276509349426	2.29662436916590	-0.14652339040204

C	-1.33846335925420	2.75644597667134	-0.32935029263228
Cl	-1.06496388964540	4.48396221435647	-0.48702322745221
C	-0.25950519994021	1.89843560759756	-0.36445968933017
C	-0.55571985831827	0.54469268690409	-0.23498213435159
C	-1.86857881478922	0.00791470663133	-0.09579306232716
C	-1.69841280891599	-1.44672900674402	-0.00798399887954
C	-0.29266262843306	-1.67544476417290	-0.04503568508526
C	0.30500470760120	-2.92641900826980	0.06205018798462
C	-0.53804782065893	-4.01606879919801	0.18125222903318
C	-1.92389233923804	-3.84069346928075	0.15737233941691
C	-2.53239731976981	-2.58943893117938	0.04983801030944
C	-4.03251033724083	-2.56530537170982	-0.06043363633777
N	0.36993758197933	-0.47362154142317	-0.20618970998622
C	1.78264356610208	-0.30259895726662	-0.18219927550027
C	2.51395467972636	-0.45498346536588	-1.35697735165595
C	3.89116551717231	-0.29648350218959	-1.35764140385813
C	4.53387098990834	0.02278758359730	-0.16279896544295
O	5.88978464556569	0.17346957326586	-0.20495865431092
C	3.80261769509903	0.17421058456657	1.01587165578299
C	2.41828918047929	0.01106134571644	1.02603901953216
C	1.62380292272533	0.16334398136352	2.29090142705930
H	-4.44841752736905	-0.02147180194642	1.17650410307377
H	-4.82221634331038	0.01814446344010	-0.54939303492641
H	-4.95421422904343	1.48850020101220	0.41568962942336
H	-3.44872999148060	3.01965275762475	-0.08568465877945
H	0.75990150258434	2.24915460285314	-0.48046177865138
H	1.38547990138750	-3.02829761461632	0.03927909602989
H	-0.12432585552540	-5.01634516520684	0.26781666430716
H	-2.56196548504914	-4.71870815393803	0.20464876065677
H	-4.35682741761798	-2.01441968450981	-0.94739069583363
H	-4.51233519976590	-2.11082833864112	0.80991197279241
H	-4.41282416119775	-3.58599353735801	-0.14887324842947

H	1.98810568112819	-0.69965264118295	-2.27536782849946
H	4.47505688680017	-0.41137546882879	-2.26455940290225
H	4.31695948565191	0.41868671947099	1.94393056691915
H	2.28031083608025	0.29113266540421	3.15460265324253
H	0.98953968933864	-0.71374426167137	2.45996969380345
H	0.95625096832084	1.03092957340048	2.23276929649356
H	6.21389559721972	0.39643510286176	0.67523004672741

Coordinates of (*S*)-**11,** Conformer #11

charge: 0, multiplicity: 1

42

C	-4.29860694149352	0.49809817257692	0.50244406138001
C	-2.86072532582313	0.84303466603606	0.22769827717449
C	-2.52529884915511	2.19677427853716	0.26567266740630
C	-1.20875730267224	2.63291157169938	0.11376022755508
Cl	-0.87553992614470	4.35566815541148	0.17392490720541
C	-0.16214323489712	1.75034495818447	-0.05429505807198
C	-0.50490189296311	0.40245727108098	-0.09578684181305
C	-1.83391856607147	-0.10326999506147	-0.00002485240567
C	-1.71534487664824	-1.56174949717715	-0.10331882845484
C	-0.31962068382828	-1.83169264638167	-0.19647301199198
C	0.23348752847776	-3.10562092190734	-0.26543446568400
C	-0.64741364985496	-4.17175414800895	-0.27418234430952
C	-2.02636542418784	-3.94704749012160	-0.25172295807313
C	-2.58992966793716	-2.67207083208994	-0.18474303112003
C	-4.08890453495427	-2.57866705330876	-0.27215918504268
N	0.38333336256239	-0.64246831110718	-0.21443656883755
C	1.80148812523790	-0.52279254363944	-0.21753669811673
C	2.48799576446788	-0.50355743394864	-1.42842291048939
C	3.86945062601622	-0.39016773159112	-1.45547192643257
C	4.56209356647541	-0.29345815573809	-0.24977692063321

O	5.920548309743 18	-0.181377028399 98	-0.318617138043 65
C	3.875538480891 79	-0.314582540616 09	0.964867714113 42
C	2.487012960671 18	-0.431394987455 77	1.000416720130 39
C	1.738540333473 87	-0.457627486967 15	2.301754769955 81
H	-4.379064345703 71	-0.233911695087 14	1.310003065927 00
H	-4.804648883932 56	0.087405208742 51	-0.374648899414 68
H	-4.844222414255 75	1.393588513793 76	0.809219784475 38
H	-3.303223428816 94	2.932172313444 39	0.439580054735 29
H	0.867397050037 65	2.078626248843 37	-0.143598962962 00
H	1.309112503254 89	-3.240266225850 31	-0.323083198126 10
H	-0.269419677624 02	-5.188408934219 55	-0.326774558018 13
H	-2.695166588096 04	-4.801159252617 21	-0.311049184630 86
H	-4.396406623635 91	-1.884097443559 04	-1.058330861053 93
H	-4.546716647819 79	-2.249257769948 61	0.664190663489 67
H	-4.506168013453 53	-3.559328162918 22	-0.514081859704 61
H	1.923981459807 11	-0.578542835240 29	-2.353696004024 48
H	4.419428564245 99	-0.372433059281 69	-2.390295717681 59
H	4.428418307259 39	-0.241638255154 39	1.900088660811 69
H	2.426644552567 27	-0.465970827038 01	3.150239709772 41
H	1.094644801603 96	-1.341629503370 53	2.365600142241 50
H	1.088563735554 61	0.418724930993 31	2.394753947345 91
H	6.281367467621 43	-0.116373521538 47	0.573066611416 53

Coordinates of (*S*)-**11,** Conformer #12

charge: 0, multiplicity: 1

42

C	-4.389365676108 72	0.541709489939 50	-0.102503153134 77
C	-2.929769220038 19	0.895888847173 89	-0.018893901809 96
C	-2.621734977019 66	2.255578804849 96	0.035869561920 12
C	-1.303620960707 55	2.713322688625 78	0.039429562721 17
Cl	-1.007454340286 41	4.441572295920 10	0.122900487218 50

C	-0.23220814500993	1.84909374102053	-0.04618859751648
C	-0.54645852061531	0.49486097405337	-0.10252134973604
C	-1.86705619950538	-0.03884741960072	-0.04519626063699
C	-1.71022790364089	-1.49799385508367	-0.07994917859230
C	-0.31091251467707	-1.73449730103403	-0.20561815800424
C	0.27226640773311	-2.99446499480454	-0.28322500602992
C	-0.57602602002941	-4.08416953252217	-0.21482002332398
C	-1.95114606999153	-3.89708815503347	-0.05025533819583
C	-2.54483158569027	-2.63682816617648	0.03221096279550
C	-4.02524305987515	-2.59412574530534	0.29633474735565
N	0.36518098922001	-0.53026118761253	-0.22363719096984
C	1.78025845026126	-0.37943277412655	-0.19969044907461
C	2.46305386256789	-0.12409613070520	-1.38289602747452
C	3.84339901347510	0.03188112964724	-1.37917050228310
C	4.53404543382038	-0.07449543678011	-0.17256083287874
O	5.88902169000733	0.06378633362712	-0.08577870034500
C	3.84837039278948	-0.32932999754067	1.01534532613158
C	2.46563708508138	-0.48182200250507	1.02087171186325
C	1.71632143729604	-0.75126368191501	2.29403019423947
H	-4.73946346431407	0.00640671390861	0.78306960714550
H	-4.59190995539170	-0.08395007320339	-0.97566136181436
H	-4.98831305312889	1.45036981460367	-0.19840941394322
H	-3.42701661834067	2.98173121004017	0.05918075096979
H	0.79455683205651	2.19573414972139	-0.07715250421717
H	1.34787260020211	-3.10113638410077	-0.38675701498122
H	-0.17348338314253	-5.09118409968642	-0.27086868924682
H	-2.58971491797169	-4.77173630066441	0.03591998768620
H	-4.25138777311642	-2.01711449507477	1.19733642914140
H	-4.40279822040140	-3.60800477463305	0.45071581803069
H	-4.58686664810229	-2.15659823216890	-0.53243251122859
H	1.90250468988609	-0.04798416388921	-2.31012465997314
H	4.37581838486395	0.23273332691529	-2.30597226740261

H	6.24796243931743	0.24279373546493	-0.96246886699312
H	4.41535895946553	-0.40022160024531	1.93894593858953
H	1.27158323461425	-1.75334060668562	2.28011240684560
H	0.89246657305212	-0.04059617708255	2.42161119376000
H	2.37791075139516	-0.67858996733149	3.16000727339257

Coordinates of (*S*)-**11,** Conformer #13

charge: 0, multiplicity: 1

42

C	-4.39160201023201	0.52743517346499	-0.33995690230238
C	-2.94344792304997	0.91530712723231	-0.21537391439821
C	-2.65117306822863	2.27830482927363	-0.27773089517147
C	-1.33777974895606	2.74923980757889	-0.27857752668190
Cl	-1.05992522590600	4.48129247637152	-0.34874790565373
C	-0.25504903726049	1.89384098372346	-0.26303744724343
C	-0.55420861646169	0.53666916321545	-0.19886084279854
C	-1.87122365081737	-0.00114093272594	-0.11190281222950
C	-1.70421615093840	-1.45385177281203	-0.00559139434814
C	-0.30336868040131	-1.69201340980289	-0.10449147462127
C	0.28447408936417	-2.95131166601634	-0.06236382033360
C	-0.56044392254277	-4.03311382806782	0.11024173236495
C	-1.93468305587324	-3.83659789649889	0.27024901920109
C	-2.53215678548316	-2.57568843749329	0.23692822790753
C	-4.00304210616138	-2.50113625573436	0.54413195395183
N	0.36527835484163	-0.48837754103183	-0.22209956681392
C	1.77943041692250	-0.32743218817860	-0.19968847003572
C	2.48090566716838	-0.25310744062470	-1.39681575367993
C	3.86104705295618	-0.09401053806096	-1.39452208866620
C	4.53171473435545	-0.01112904331486	-0.17496283719653
O	5.88472632824379	0.14468551335729	-0.08893812532828
C	3.82707926464480	-0.08564416244900	1.02690501211327

C	2.44509603030504	-0.24310459258598	1.03308828695813
C	1.67275946164959	-0.31625698178640	2.31875458110684
H	-4.98303120329529	1.39359225100822	-0.64643146368924
H	-4.81035323146809	0.15872046570584	0.60004564423449
H	-4.52295663819460	-0.25158086228432	-1.09494810213858
H	-3.46351549354069	2.99299954034472	-0.35442042069646
H	0.76804902152652	2.24940969994847	-0.31239964395972
H	1.36072982409654	-3.06384559257720	-0.15101307620393
H	-0.15338205878305	-5.03909341345709	0.14974322666406
H	-2.56764754386448	-4.69987010343620	0.45640559697507
H	-4.35389459898615	-3.47024371602876	0.90772321136314
H	-4.60560791141992	-2.24144962449512	-0.33034894874691
H	-4.20559991933419	-1.76088152045626	1.32283043621530
H	1.93545722122233	-0.32105350354426	-2.33362946369838
H	4.40847766428587	-0.03496380932239	-2.33244480516118
H	6.25750957084650	0.19021418570806	-0.97685493665033
H	4.37906790614967	-0.01554752818117	1.95958889733393
H	0.93885751692717	0.49570135609413	2.37832951781504
H	2.33945709504547	-0.24454679330546	3.18083467471022
H	1.11341136064737	-1.25613941875486	2.38624261953259

4.3 Mechanistic computations

Table S6: Energies of intermediates and transition states for the mechanistic calculations at the ωB97M-V/def2-TZVPP/SMD(acetonitrile)//TPSS-D4/def2-SVP level of theory.

Structure	Electronic energy [E_h]	Zero Point Energy [E_h]	Correction to	
			Enthalpy [E_h]	Gibbs free energy [E_h]
I-2a	-3501.602140	0.609025	0.660751	0.531075
I-2b	-3501.602287	0.609099	0.661192	0.530725
TS_{rot}	-3501.584231	0.608997	0.660374	0.531325
$TS_{RE,1}$	-3501.578062	0.608329	0.660028	0.529881
$TS_{RE,2}$	-3501.575326	0.608557	0.660150	0.530365
(*S*)-**P-1**_Pd-L	-3501.644545	0.610695	0.662753	0.532479
(*R*)-**P-1**_Pd-L	-3501.643348	0.611572	0.663390	0.534284

Coordinates of **I-2a**

charge: 0, multiplicity: 1

85

C	4.27020	-0.19982	-2.69547
C	4.12868	-1.32701	-1.69157
C	4.57816	-2.60583	-2.07076
C	4.38093	-3.70813	-1.23052
C	3.65423	-3.57018	-0.04681
C	3.14782	-2.30801	0.34163
N	2.21829	-2.20289	1.38007
C	2.24937	-2.98240	2.52634
C	1.02519	-3.35439	3.16300
C	1.06092	-4.19239	4.28940
C	2.27091	-4.65436	4.82189
C	3.47733	-4.26502	4.21403
C	3.47033	-3.43982	3.08983
C	3.49347	-1.15003	-0.43327

C	3.15195	0.19069	0.11152
C	4.10437	1.25649	0.14684
C	3.71876	2.52460	0.62020
C	2.44040	2.72346	1.14289
Cl	1.96482	4.31647	1.71557
C	1.52799	1.66677	1.23784
C	1.88824	0.42641	0.69978
H	3.77883	0.72306	-2.35314
H	3.80937	-0.50106	-3.65387
H	5.32822	0.03402	-2.90855
H	5.07115	-2.73458	-3.04080
H	4.74608	-4.69770	-1.52726
H	3.41788	-4.44553	0.56516
H	0.11400	-4.48323	4.76005
H	2.27439	-5.30077	5.70506
H	4.43431	-4.60248	4.62740
H	4.43183	3.35338	0.60970
H	0.55186	1.84523	1.69330
C	5.56139	1.07338	-0.22709
H	5.80597	1.57498	-1.18032
H	5.82754	0.01024	-0.32151
H	6.20043	1.52665	0.55043
Pd	0.60658	-1.08755	0.87943
C	-0.28475	-2.83439	2.63969
F	-6.38032	0.88228	3.87680
C	-5.70652	1.94725	3.37446
C	-4.57128	1.50590	2.47923
C	-3.29679	1.28304	3.02367
C	-2.26360	0.82020	2.20110
C	-4.81058	1.27224	1.11459
C	-3.77483	0.81536	0.29289
C	-2.49328	0.58860	0.83091

P	-1.07606	0.02486	-0.19692
C	-1.87589	-0.95562	-1.53303
C	-2.14131	-2.31926	-1.29828
C	-2.76649	-3.09758	-2.27632
C	-3.12310	-2.51817	-3.50560
C	-3.84176	-3.34573	-4.54585
F	-3.59324	-2.90370	-5.80093
F	-3.48035	-4.64885	-4.48909
F	-5.18682	-3.29916	-4.36781
C	-2.84981	-1.16444	-3.75436
C	-2.23013	-0.38458	-2.77027
C	-0.47937	1.54257	-1.03438
C	-0.89614	2.82434	-0.64104
C	-0.19456	3.95717	-1.07714
C	0.91719	3.80642	-1.91406
C	1.75718	4.99700	-2.30659
F	2.00288	5.01129	-3.64243
F	1.16747	6.17147	-1.98930
F	2.96637	4.97172	-1.69124
C	1.30636	2.52873	-2.35637
C	0.61800	1.40112	-1.91259
F	-6.60655	2.70549	2.70474
F	-5.26305	2.67033	4.42886
H	-3.11602	1.47243	4.08537
H	-1.26767	0.63335	2.61912
H	-5.80564	1.45409	0.69861
H	-3.96434	0.63179	-0.76945
H	-1.84644	-2.77538	-0.34691
H	-2.96464	-4.15777	-2.09580
H	-3.11586	-0.72429	-4.71956
H	-2.01227	0.66984	-2.96745
H	-1.73983	2.94329	0.04535

H	-0.49207	4.95348	-0.74227
H	2.16807	2.42014	-3.02080
H	0.96379	0.40318	-2.20275
H	4.41005	-3.13288	2.62126
H	-0.32389	-2.90480	1.51036
H	-0.45992	-1.77460	2.92284
H	-1.14957	-3.41461	3.00298

Coordinates of **I-2b**

charge: 0, multiplicity: 1

85

C	-4.19458	-2.21300	1.21949
C	-3.35583	-2.90570	0.16488
C	-3.10766	-4.28715	0.31851
C	-2.27076	-4.96624	-0.57188
C	-1.60233	-4.26613	-1.58172
C	-1.78476	-2.87364	-1.72626
N	-1.06412	-2.12814	-2.67236
C	0.28033	-2.41755	-2.93635
C	0.81189	-2.03848	-4.21875
C	2.18410	-2.17440	-4.43946
C	3.06181	-2.65360	-3.44216
C	2.56404	-2.99680	-2.18542
C	1.18569	-2.86826	-1.91513
C	-2.75244	-2.19808	-0.90564
C	-3.01735	-0.75060	-1.15781
C	-4.34214	-0.24906	-1.31025
C	-4.54826	1.13597	-1.47670
C	-3.46185	2.00596	-1.56410
Cl	-3.73789	3.73593	-1.73738
C	-2.14618	1.52386	-1.53450

C	-1.93885	0.16027	-1.31999
H	-3.87578	-2.54099	2.22494
H	-5.26528	-2.46777	1.12477
H	-4.10027	-1.11725	1.16637
H	-3.57592	-4.82397	1.15115
H	-2.10972	-6.04434	-0.46234
H	-0.91546	-4.78456	-2.25777
H	2.58746	-1.89940	-5.42082
H	4.12990	-2.75484	-3.66106
H	3.23270	-3.36880	-1.40196
H	-5.56476	1.53028	-1.56597
H	-1.31450	2.21885	-1.66658
C	-5.55969	-1.14838	-1.37809
H	-6.18550	-1.05566	-0.47214
H	-5.27981	-2.20613	-1.49440
H	-6.18959	-0.85857	-2.23717
Pd	-0.11416	-0.67244	-1.49850
C	-0.12753	-1.50429	-5.26584
F	-0.16966	-4.63003	4.62918
C	0.32391	-3.42621	5.00338
C	0.48942	-2.49574	3.82507
C	-0.37626	-2.59932	2.72534
C	-0.24760	-1.70776	1.65502
C	1.48441	-1.50403	3.85051
C	1.60935	-0.61015	2.78112
C	0.74129	-0.70323	1.67685
P	0.83494	0.44101	0.23033
C	-0.03242	1.95123	0.79812
C	-1.15825	1.82946	1.63409
C	-1.98025	2.93450	1.87438
C	-1.68355	4.17069	1.28118
C	-2.56039	5.36820	1.55874

F	-2.55528	6.24837	0.53135
F	-3.84383	5.01101	1.79184
F	-2.13351	6.04499	2.65905
C	-0.55769	4.30385	0.45389
C	0.26203	3.19755	0.20934
C	2.60323	0.92292	0.11732
C	3.38476	0.27026	-0.85540
C	4.74772	0.56073	-0.97781
C	5.33506	1.51711	-0.13452
C	6.79287	1.87721	-0.30337
F	7.51557	0.83696	-0.78162
F	6.95076	2.90471	-1.17525
F	7.35358	2.26254	0.86778
C	4.56123	2.17976	0.83288
C	3.19936	1.88427	0.95887
F	-0.53582	-2.91342	5.92054
F	1.49814	-3.64506	5.64265
H	-1.13820	-3.38316	2.68927
H	-0.91537	-1.79815	0.79015
H	2.16630	-1.44045	4.70326
H	2.39577	0.15001	2.80512
H	-1.41132	0.86048	2.07465
H	-2.86829	2.83257	2.50399
H	-0.34170	5.26540	-0.01964
H	1.11853	3.29914	-0.46548
H	2.91944	-0.47049	-1.51569
H	5.35468	0.04631	-1.72801
H	5.02814	2.92049	1.48834
H	2.59745	2.40936	1.70768
H	0.77883	-3.21902	-0.96095
H	-0.61927	-0.58258	-4.90610
H	-0.93991	-2.22375	-5.46742

H	0.40656	-1.28642	-6.20479

Coordinates of **TS_{rot}**

charge: 0, multiplicity: 1, imaginary frequency at 63.77 *i*cm^{-1}

85

C	3.89789	0.05510	2.63905
C	3.91123	0.98035	1.43944
C	4.45252	2.26991	1.61368
C	4.43267	3.19073	0.56580
C	3.80641	2.87771	-0.64606
C	3.21656	1.61092	-0.85846
N	2.41803	1.28258	-1.96991
C	2.67995	1.52529	-3.33289
C	3.22232	2.74417	-3.81458
C	3.45953	2.96067	-5.17681
C	3.13856	1.97587	-6.11685
C	2.58493	0.77268	-5.66016
C	2.35464	0.51917	-4.29805
C	3.36447	0.61878	0.18241
C	2.89478	-0.77400	-0.08015
C	3.71605	-1.91755	0.14223
C	3.17943	-3.20817	-0.04537
C	1.87268	-3.37303	-0.50587
Cl	1.20115	-4.98642	-0.69288
C	1.07836	-2.26722	-0.84377
C	1.61346	-0.99809	-0.62147
H	3.25875	-0.82598	2.48295
H	3.52018	0.59765	3.52279
H	4.91300	-0.29809	2.89452
H	4.87776	2.54580	2.58508
H	4.86112	4.18988	0.70298

H	3.71964	3.65498	-1.40291
H	3.88421	3.91851	-5.49774
H	3.31306	2.13806	-7.18537
H	2.33502	-0.01554	-6.38068
C	1.79562	-0.81678	-3.88418
H	3.79814	-4.08954	0.14639
H	0.08527	-2.42195	-1.27104
C	5.18067	-1.81030	0.50853
H	5.55413	-0.78263	0.38722
H	5.77456	-2.47876	-0.13878
H	5.36104	-2.12204	1.55268
Pd	0.65481	0.62532	-1.21476
H	3.44754	3.55162	-3.12056
H	0.80749	-0.71238	-3.38820
H	2.45001	-1.31926	-3.15129
H	1.66866	-1.47403	-4.76011
F	2.09554	0.07954	6.02663
C	1.54215	-1.03833	5.49574
C	0.79921	-0.74526	4.21543
C	0.53735	-1.79068	3.31475
C	-0.12521	-1.52767	2.11361
C	0.37245	0.55809	3.92422
C	-0.29087	0.82248	2.72104
C	-0.53516	-0.21413	1.80156
P	-1.13131	0.18270	0.10787
C	-2.27881	-1.17571	-0.33480
C	-2.40848	-1.49889	-1.69996
C	-3.27301	-2.52083	-2.10554
C	-4.00950	-3.23128	-1.14426
C	-4.89784	-4.37795	-1.57111
F	-4.22402	-5.55383	-1.56072
F	-5.96022	-4.52122	-0.74321

F	-5.37502	-4.20244	-2.82532
C	-3.88808	-2.91505	0.21867
C	-3.02557	-1.89017	0.62296
C	-2.20795	1.65987	0.33153
C	-1.59807	2.92654	0.21932
C	-2.35171	4.09298	0.38942
C	-3.72663	3.99889	0.65668
C	-4.55750	5.25565	0.77992
F	-5.05511	5.63836	-0.42216
F	-5.61392	5.07824	1.60832
F	-3.83022	6.29260	1.25754
C	-4.34352	2.74142	0.75999
C	-3.58696	1.57552	0.59922
F	2.54419	-1.92977	5.29265
F	0.72943	-1.56934	6.44313
H	0.87733	-2.80594	3.53821
H	-0.29578	-2.34469	1.40826
H	0.58052	1.36938	4.62672
H	-0.60007	1.84675	2.49266
H	-1.81604	-0.95017	-2.44148
H	-3.37553	-2.77048	-3.16512
H	-4.47171	-3.46915	0.95927
H	-2.92721	-1.65113	1.68666
H	-0.52434	2.99449	0.00132
H	-1.87540	5.07440	0.31394
H	-5.41452	2.67780	0.97235
H	-4.07417	0.59902	0.67769

Coordinates of $\mathbf{TS_{RE,1}}$

charge: 0, multiplicity: 1, imaginary frequency at 282.77 *i*cm^{-1}

85

C	-2.18709	-3.88622	1.38053
C	-2.66380	-3.45647	0.01089
C	-2.92558	-4.43740	-0.96627
C	-3.21504	-4.09649	-2.29533
C	-3.15339	-2.76100	-2.71297
C	-2.86265	-1.77134	-1.76312
N	-2.58303	-0.42749	-2.11946
C	-3.53557	0.37925	-2.76959
C	-3.12566	1.49835	-3.54457
C	-4.12036	2.28626	-4.14922
C	-5.48413	1.99503	-4.01029
C	-5.87726	0.88919	-3.24221
C	-4.91154	0.09523	-2.61942
C	-2.74350	-2.09480	-0.37379
C	-2.68936	-0.86641	0.44130
C	-3.31939	-0.60368	1.68850
C	-3.36855	0.72440	2.15949
C	-2.88237	1.78401	1.38028
Cl	-2.96820	3.42310	2.00686
C	-2.32878	1.57306	0.11157
C	-2.18721	0.23923	-0.29647
H	-3.00128	-4.26785	2.02085
H	-1.69677	-3.05723	1.90920
H	-1.45012	-4.70170	1.27651
H	-2.87066	-5.49404	-0.68028
H	-3.42679	-4.88384	-3.02663
H	-3.28704	-2.48363	-3.76263
H	-3.80966	3.14690	-4.75304
H	-6.23284	2.62833	-4.49689
H	-6.93889	0.65104	-3.11646
H	-3.84868	0.94515	3.11677
H	-1.98882	2.41431	-0.49568

C	-4.02991	-1.66580	2.49471
H	-3.34574	-2.18404	3.18942
H	-4.47735	-2.42776	1.83642
H	-4.83286	-1.21003	3.09684
Pd	-0.60440	-0.08254	-1.57032
C	-1.66787	1.82420	-3.74666
F	-1.36146	-3.55471	4.67969
C	-0.14459	-2.96548	4.86988
C	0.28571	-2.19494	3.64809
C	1.22647	-2.73340	2.75712
C	1.56120	-2.03680	1.58887
C	-0.31622	-0.95518	3.37344
C	0.00644	-0.26811	2.20193
C	0.95107	-0.80249	1.30009
P	1.22473	0.09253	-0.28624
C	1.61332	1.80056	0.27926
C	1.25442	2.87074	-0.56155
C	1.50601	4.19183	-0.17691
C	2.11350	4.45164	1.06158
C	2.32906	5.87782	1.51172
F	3.42011	5.99237	2.30720
F	2.49832	6.71640	0.46180
F	1.27065	6.33920	2.22242
C	2.47480	3.39159	1.90905
C	2.22439	2.07125	1.51982
C	2.82959	-0.58595	-0.88643
C	4.08352	-0.06441	-0.51709
C	5.25934	-0.64624	-1.00445
C	5.19019	-1.75832	-1.85907
C	6.45838	-2.35417	-2.42345
F	6.32555	-3.68012	-2.66620
F	6.80159	-1.76915	-3.59877

F	7.50730	-2.19483	-1.58145
C	3.94358	-2.28634	-2.23263
C	2.76939	-1.69399	-1.75597
F	-0.27259	-2.16390	5.95430
F	0.72213	-3.95326	5.18946
H	1.69721	-3.69481	2.97946
H	2.29882	-2.46064	0.90056
H	-1.04873	-0.53226	4.06669
H	-0.48245	0.68716	1.98713
H	0.76333	2.65642	-1.51752
H	1.22804	5.02199	-0.83211
H	2.95161	3.60253	2.87052
H	2.49269	1.24842	2.19017
H	4.14474	0.80119	0.14936
H	6.23425	-0.24301	-0.71591
H	3.89556	-3.15440	-2.89617
H	1.79093	-2.08846	-2.05648
H	-5.20575	-0.76043	-2.00399
H	-1.12583	0.97137	-4.20063
H	-1.15704	2.03888	-2.78534
H	-1.54590	2.70199	-4.40227

Coordinates of **$TS_{RE,2}$**

charge: 0, multiplicity: 1, imaginary frequency at 240.70 *i*cm^{-1}

85

C	-2.91964	-4.30737	0.00434
C	-3.28199	-3.35397	-1.11527
C	-3.72887	-3.87992	-2.34416
C	-3.93852	-3.05886	-3.46173
C	-3.60406	-1.69941	-3.41717
C	-3.11954	-1.16387	-2.21395

N	-2.57476	0.12665	-2.10947
C	-3.17290	1.30074	-2.60722
C	-2.35165	2.24396	-3.26247
C	-2.87380	3.45058	-3.73667
C	-4.23928	3.72355	-3.57115
C	-5.05568	2.79547	-2.90927
C	-4.55262	1.58533	-2.39972
C	-3.08177	-1.95534	-1.01886
C	-2.84958	-1.10550	0.16431
C	-3.51252	-1.18046	1.42326
C	-3.39865	-0.10163	2.32097
C	-2.71844	1.06761	1.95602
Cl	-2.61108	2.38832	3.11032
C	-2.12978	1.21634	0.69564
C	-2.15702	0.09729	-0.14672
H	-2.31358	-5.13691	-0.40072
H	-3.80558	-4.75885	0.48461
H	-2.32672	-3.80363	0.78363
H	-3.89034	-4.96049	-2.43020
H	-4.30371	-3.49586	-4.39732
H	-3.67232	-1.06363	-4.30496
H	-2.22055	4.16770	-4.24484
H	-4.66664	4.66009	-3.94413
H	-6.11654	3.02448	-2.75433
C	-5.44541	0.65491	-1.61524
H	-3.88748	-0.15010	3.29663
H	-1.63705	2.14886	0.41329
C	-4.44519	-2.30918	1.79982
H	-3.91489	-3.14881	2.28327
H	-4.96065	-2.70831	0.91110
H	-5.20527	-1.94765	2.51128
Pd	-0.60782	0.01121	-1.50038

H	-1.29184	1.99399	-3.39394
H	-5.69690	-0.25600	-2.18779
H	-6.38568	1.16247	-1.34516
H	-4.94750	0.32297	-0.68813
F	6.61902	-4.01303	-1.35685
C	5.39454	-4.55407	-1.13060
C	4.35552	-3.48310	-0.89537
C	4.11863	-3.01281	0.40608
C	3.19239	-1.98499	0.61884
C	3.65691	-2.93515	-1.98396
C	2.72605	-1.91431	-1.76777
C	2.49407	-1.42348	-0.46800
P	1.27742	-0.05674	-0.26662
C	0.80293	-0.15790	1.50541
C	0.05545	-1.28595	1.90755
C	-0.47445	-1.35231	3.19548
C	-0.27484	-0.28616	4.09147
C	-0.88227	-0.36813	5.46942
F	-0.75463	0.78474	6.16177
F	-2.20743	-0.66629	5.41439
F	-0.30124	-1.34941	6.20955
C	0.46978	0.83316	3.70104
C	1.01089	0.89630	2.40948
C	2.31383	1.46407	-0.35258
C	1.68009	2.65807	-0.75080
C	2.39611	3.85891	-0.79548
C	3.75825	3.86964	-0.45370
C	4.52440	5.17175	-0.45543
F	4.03718	6.04186	-1.37134
F	4.45431	5.78733	0.75235
F	5.83784	4.98320	-0.72675
C	4.40195	2.68094	-0.07261

C	3.68117	1.48252	-0.01926
F	5.09566	-5.31837	-2.20766
F	5.51879	-5.37906	-0.06380
H	4.65404	-3.45649	1.25035
H	3.00259	-1.62469	1.63501
H	3.83124	-3.32081	-2.99236
H	2.16117	-1.49948	-2.61040
H	-0.13537	-2.09669	1.19663
H	-1.06882	-2.21856	3.49993
H	0.60872	1.66277	4.39812
H	1.57647	1.78122	2.10323
H	0.62092	2.62967	-1.03593
H	1.90484	4.78448	-1.10847
H	5.46721	2.69539	0.17492
H	4.18772	0.55806	0.27522

Coordinates of (*S*)-**P-1**_Pd-L

charge: 0, multiplicity: 1

85

C	1.72044	3.82801	1.52803
C	2.30233	3.55341	0.16231
C	2.30654	4.60444	-0.77333
C	2.68159	4.42971	-2.12003
C	3.03813	3.16613	-2.59716
C	3.04932	2.11658	-1.66919
N	3.30036	0.77652	-1.94405
C	3.68164	0.22061	-3.20788
C	2.68995	-0.26685	-4.08880
C	3.12388	-0.82825	-5.30528
C	4.48469	-0.89233	-5.63671
C	5.45177	-0.39415	-4.75101

C	5.04600	0.16205	-3.53110
C	2.74778	2.27326	-0.27583
C	2.88009	0.94354	0.32546
C	2.91726	0.41106	1.65022
C	3.01302	-0.98067	1.80189
C	3.13286	-1.84925	0.69229
Cl	3.40887	-3.56711	1.02005
C	3.31512	-1.36717	-0.63683
C	3.14850	0.04311	-0.76123
H	1.00174	3.04100	1.81192
H	1.18341	4.78959	1.51676
H	2.49019	3.87802	2.31633
H	1.95578	5.58905	-0.44471
H	2.65551	5.28409	-2.80472
H	3.28377	2.98816	-3.64804
H	2.37425	-1.21668	-6.00373
H	4.79045	-1.33281	-6.59174
H	6.51564	-0.44126	-5.00511
H	3.01780	-1.41080	2.80659
H	3.75725	-1.97402	-1.43356
C	2.95202	1.24963	2.90423
H	3.20809	0.61854	3.76926
H	1.98382	1.72550	3.11921
H	3.70418	2.05244	2.81881
Pd	1.14073	-1.59149	-0.70843
C	1.23077	-0.18877	-3.73400
F	0.68343	-0.45309	6.71458
C	1.05286	-1.46596	5.89337
C	0.39164	-1.39111	4.54673
C	0.00572	-0.14909	4.02573
C	-0.48369	-0.06277	2.71632
C	0.24643	-2.56052	3.77657

C	-0.23538	-2.46939	2.47151
C	-0.58614	-1.21687	1.92061
P	-0.89695	-1.14842	0.10648
C	-2.50384	-2.02440	-0.11198
C	-2.87364	-2.36794	-1.42882
C	-4.08532	-3.01638	-1.67802
C	-4.93361	-3.34136	-0.60355
C	-6.24979	-4.01560	-0.88816
F	-7.17046	-3.13933	-1.37773
F	-6.12404	-4.99669	-1.81957
F	-6.79652	-4.57860	0.21595
C	-4.57073	-3.01405	0.71132
C	-3.35887	-2.35436	0.95534
C	-1.37491	0.61084	-0.18038
C	-2.57220	1.18138	0.29235
C	-2.81448	2.54908	0.11294
C	-1.86870	3.34317	-0.55906
C	-2.06992	4.82878	-0.69547
F	-1.34896	5.51778	0.23690
F	-1.66118	5.28854	-1.90567
F	-3.36231	5.20044	-0.53812
C	-0.69090	2.77467	-1.06738
C	-0.44768	1.41408	-0.86612
F	2.41573	-1.39428	5.78331
F	0.78706	-2.62807	6.54015
H	0.10248	0.75461	4.63371
H	-0.75982	0.91510	2.31226
H	0.53357	-3.53131	4.19087
H	-0.30912	-3.37529	1.85990
H	-2.20274	-2.12877	-2.26189
H	-4.36665	-3.28241	-2.70150
H	-5.23124	-3.27255	1.54364

H	-3.08271	-2.09946	1.98325
H	-3.31262	0.56603	0.81397
H	-3.73573	2.99852	0.49436
H	0.03619	3.38775	-1.60591
H	0.47435	0.95418	-1.23415
H	5.77780	0.55221	-2.81701
H	0.91208	0.85564	-3.57195
H	1.02119	-0.73679	-2.77652
H	0.60377	-0.63244	-4.52266

Coordinates of (*R*)-**P-1**_Pd-L

charge: 0, multiplicity: 1

85

C	-4.80460	2.74858	-0.46479
C	-3.54507	3.28062	0.17644
C	-3.19777	4.61516	-0.10564
C	-2.05916	5.24599	0.43287
C	-1.21536	4.55179	1.29781
C	-1.54544	3.21808	1.57932
N	-0.83318	2.36340	2.40839
C	0.48432	2.54540	2.92258
C	1.54826	2.70227	1.98237
C	2.89192	2.65278	2.45877
C	3.12880	2.47061	3.84864
C	2.06481	2.40644	4.74860
C	0.71804	2.44857	4.30533
C	-2.68824	2.53557	1.04112
C	-2.62835	1.15971	1.56999
C	-3.36510	-0.05552	1.42518
C	-2.93475	-1.18647	2.14025
C	-1.78196	-1.16393	2.94151

Cl	-1.32055	-2.61876	3.81828
C	-0.99673	-0.02601	3.06859
C	-1.46298	1.11309	2.39931
H	-5.30641	3.55376	-1.02478
H	-5.51399	2.36269	0.28501
H	-4.58905	1.93077	-1.17162
H	-3.85034	5.18450	-0.77647
H	-1.84185	6.28731	0.17293
H	-0.33019	5.01572	1.74174
H	3.72276	2.90767	1.79162
H	4.15995	2.42906	4.21473
H	2.26423	2.31569	5.82182
C	-0.41810	2.36825	5.29581
H	-3.49696	-2.11777	2.05038
H	-0.07789	-0.01581	3.65695
C	-4.56766	-0.25112	0.53316
H	-4.33382	0.00169	-0.51332
H	-5.42214	0.37074	0.84553
H	-4.88358	-1.30537	0.56146
Pd	2.20972	0.63960	1.60924
H	1.31352	3.03042	0.96364
H	-0.13256	2.85360	6.24399
H	-0.67882	1.31861	5.52813
H	-1.32624	2.85431	4.90363
F	-3.75627	-4.70883	-1.37996
C	-3.18162	-4.55586	-0.16066
C	-2.02521	-3.59480	-0.19314
C	-2.08229	-2.47404	-1.03570
C	-1.03336	-1.54973	-1.03500
C	-0.91953	-3.79217	0.64927
C	0.11779	-2.85537	0.65957
C	0.07473	-1.72970	-0.18499

P	1.52338	-0.58330	-0.14505
C	2.77385	-1.54481	-1.10164
C	2.41382	-2.46501	-2.10656
C	3.40267	-3.14390	-2.82363
C	4.76008	-2.90229	-2.54269
C	5.80666	-3.65660	-3.32141
F	7.06684	-3.26821	-3.01579
F	5.73707	-4.99580	-3.09174
F	5.65113	-3.49147	-4.66205
C	5.12877	-1.98698	-1.54622
C	4.13312	-1.31518	-0.82529
C	1.03125	0.74198	-1.32746
C	-0.08653	1.52980	-0.97987
C	-0.46323	2.62010	-1.76267
C	0.29246	2.94869	-2.90243
C	-0.07269	4.17369	-3.69413
F	0.45642	5.30591	-3.14860
F	0.37166	4.11781	-4.97387
F	-1.41639	4.36881	-3.74198
C	1.40516	2.17280	-3.26105
C	1.77001	1.06764	-2.47928
F	-4.17773	-4.12995	0.67600
F	-2.82092	-5.78726	0.27314
H	-2.94058	-2.32640	-1.69738
H	-1.08162	-0.69258	-1.71104
H	-0.87654	-4.66529	1.30498
H	0.96976	-3.00161	1.33244
H	1.35930	-2.65310	-2.33130
H	3.12003	-3.85860	-3.60310
H	6.18477	-1.80461	-1.33019
H	4.40630	-0.60490	-0.03499
H	-0.67160	1.27864	-0.09145

H	-1.33848	3.21564	-1.48816
H	1.98551	2.42496	-4.15342
H	2.63693	0.46741	-2.77128

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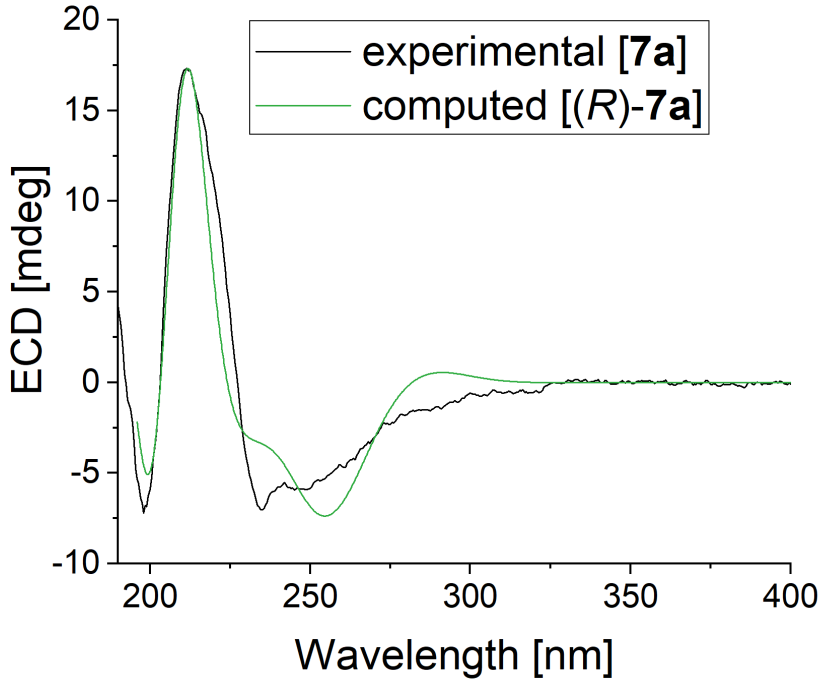
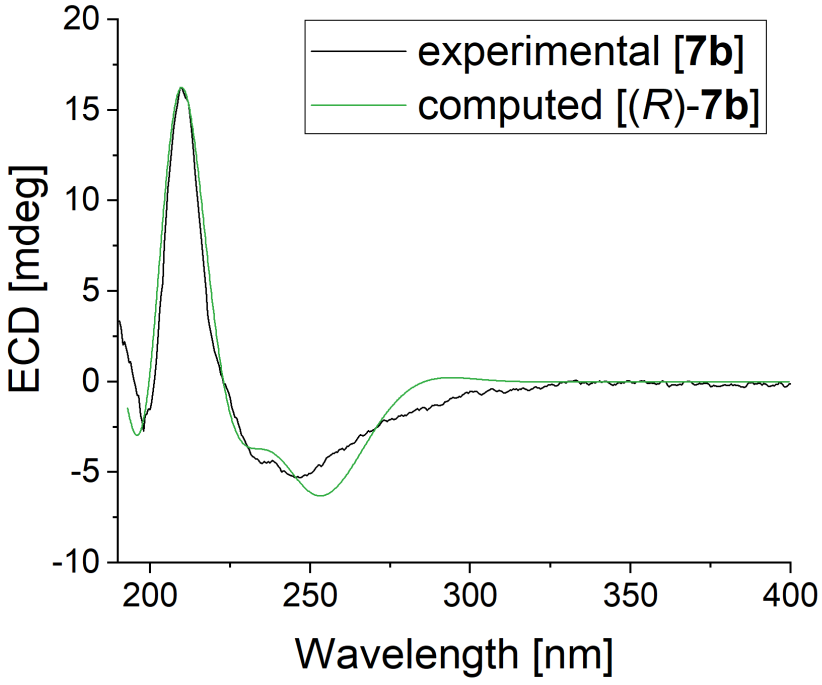
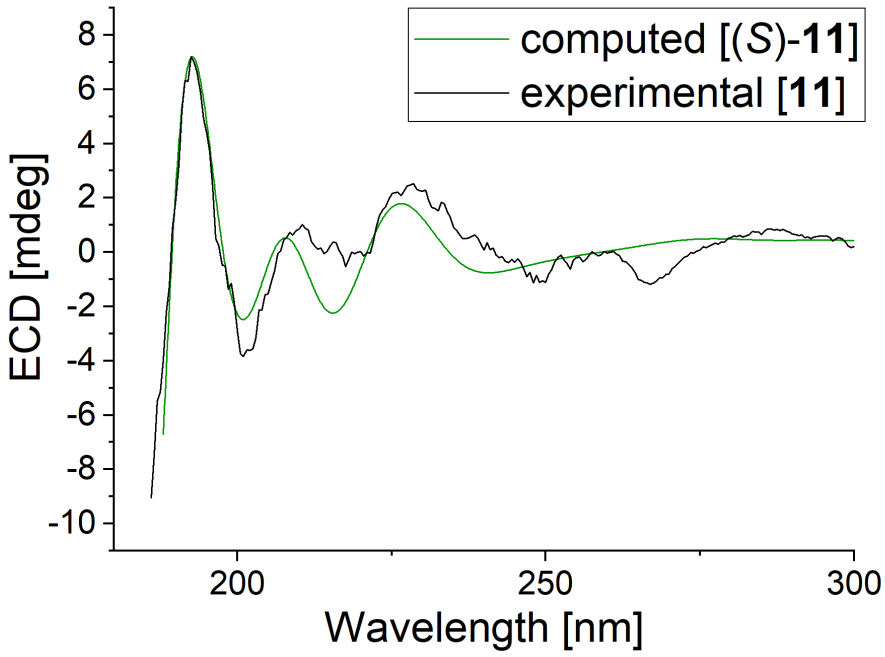
6. ECD-Spectra



Experimental and computed ECD-spectra of **7a**.

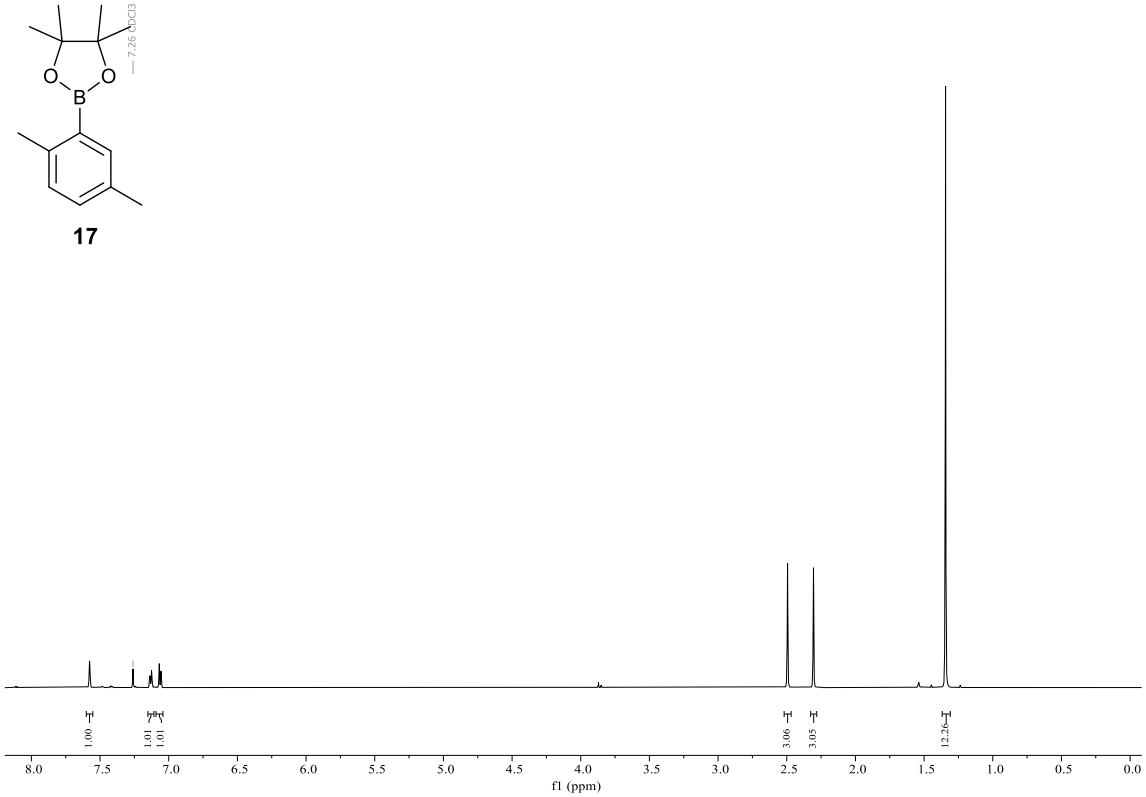


Experimental and computed ECD-spectra of **7b**.

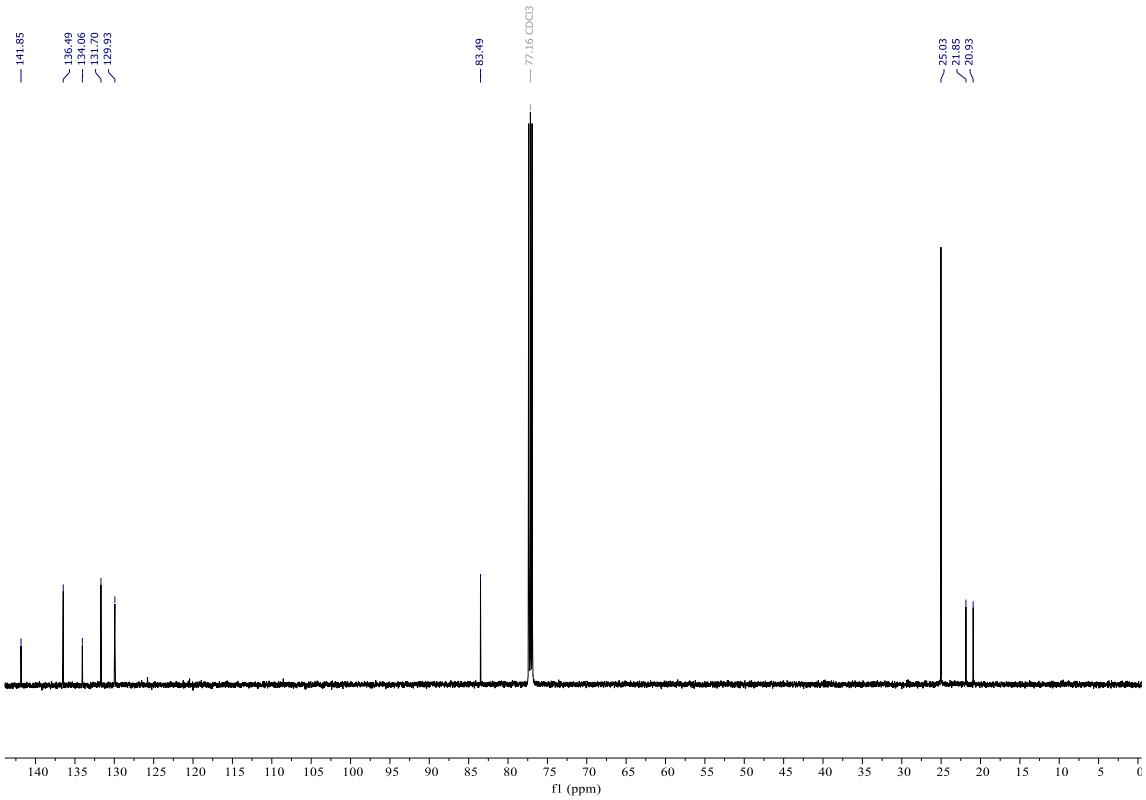


Experimental and computed ECD-spectra of **11**.

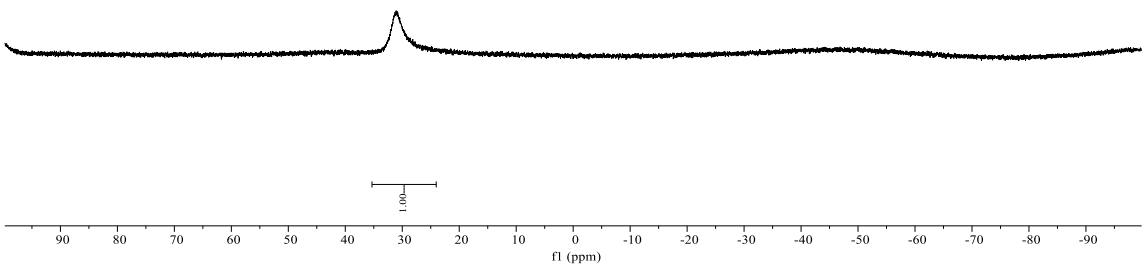
7. NMR-Spectra



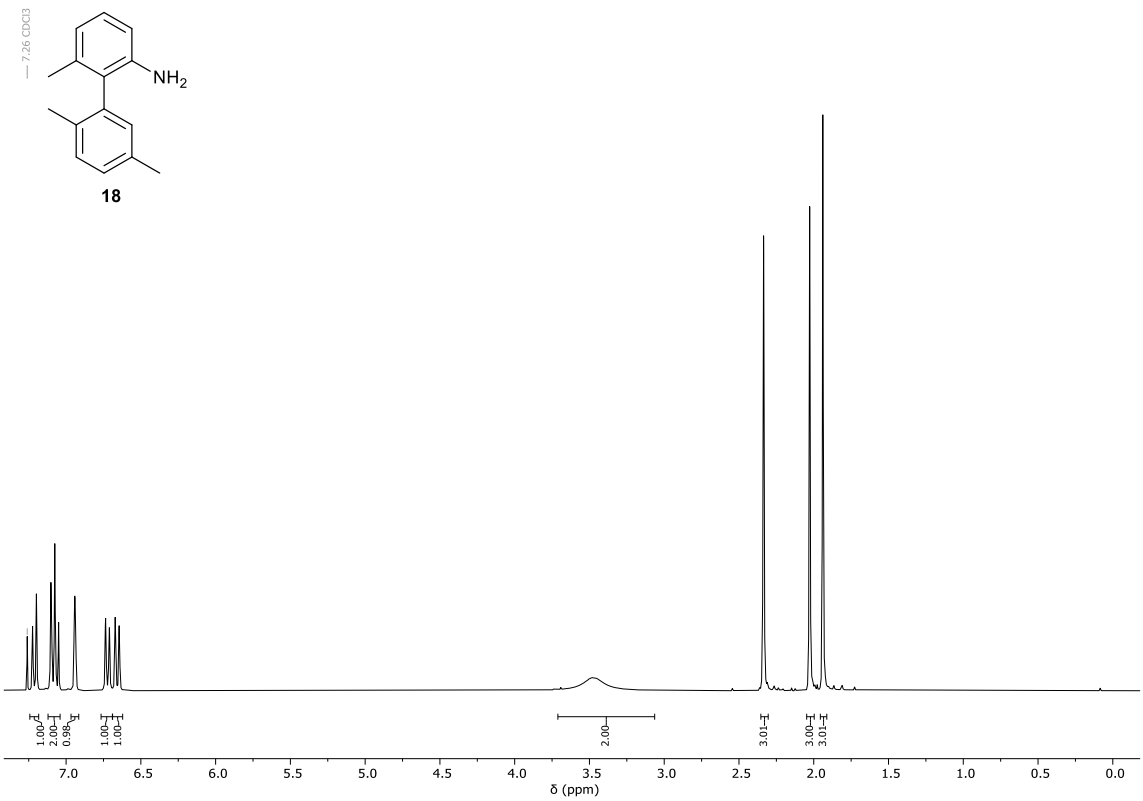
^{1}H-NMR spectrum of **17**. 600 MHz, $CDCl_3$



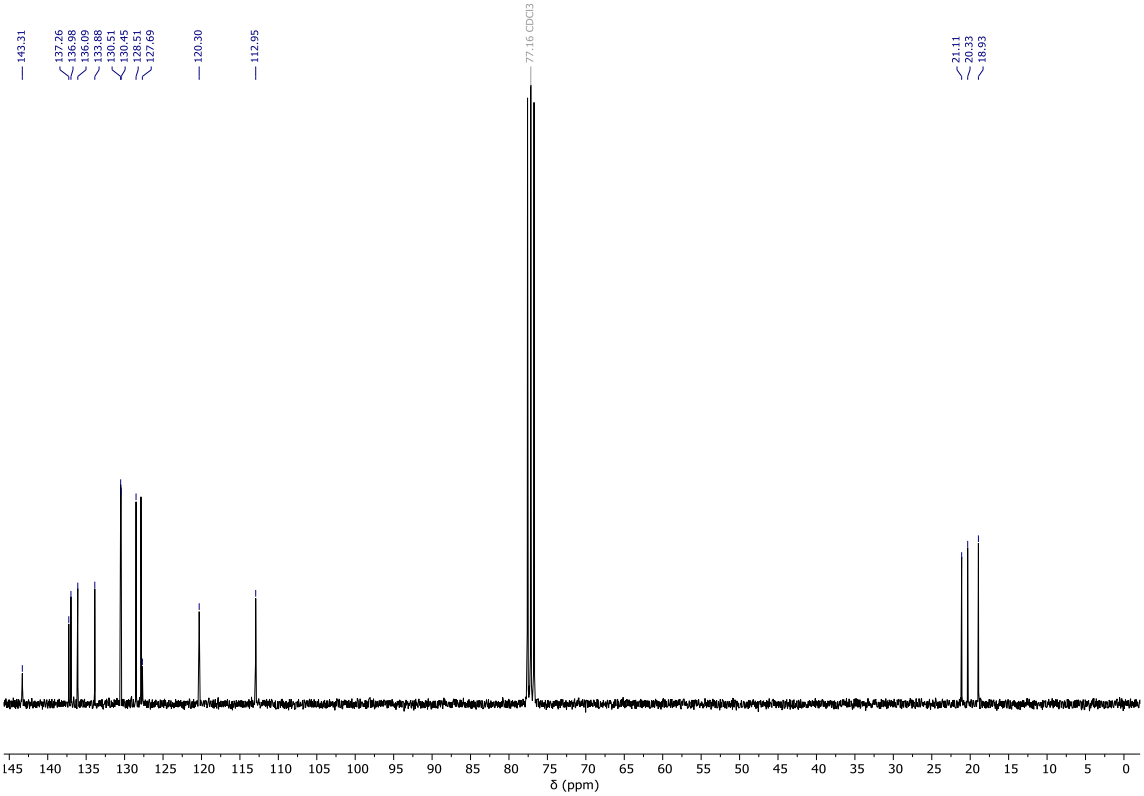
^{13}C-NMR spectrum of **17**. 151 MHz, $CDCl_3$



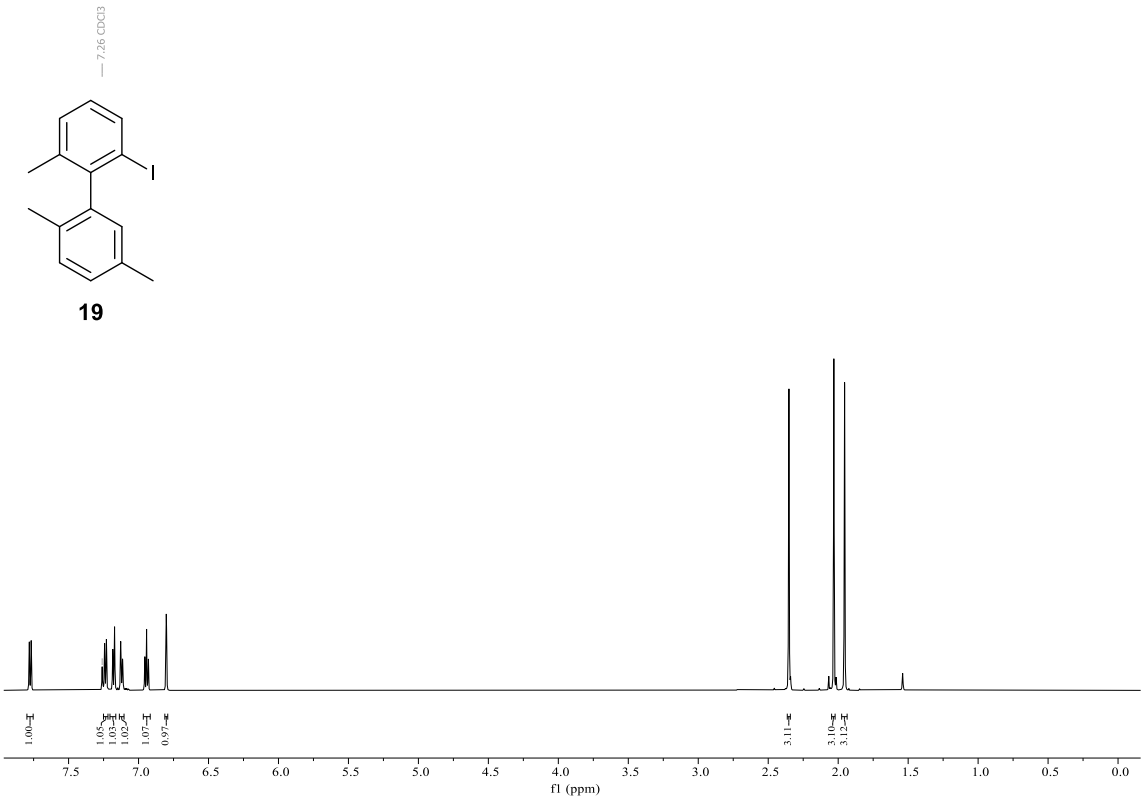
^{11}B-NMR spectrum of **17**. 96 MHz, $CDCl_3$



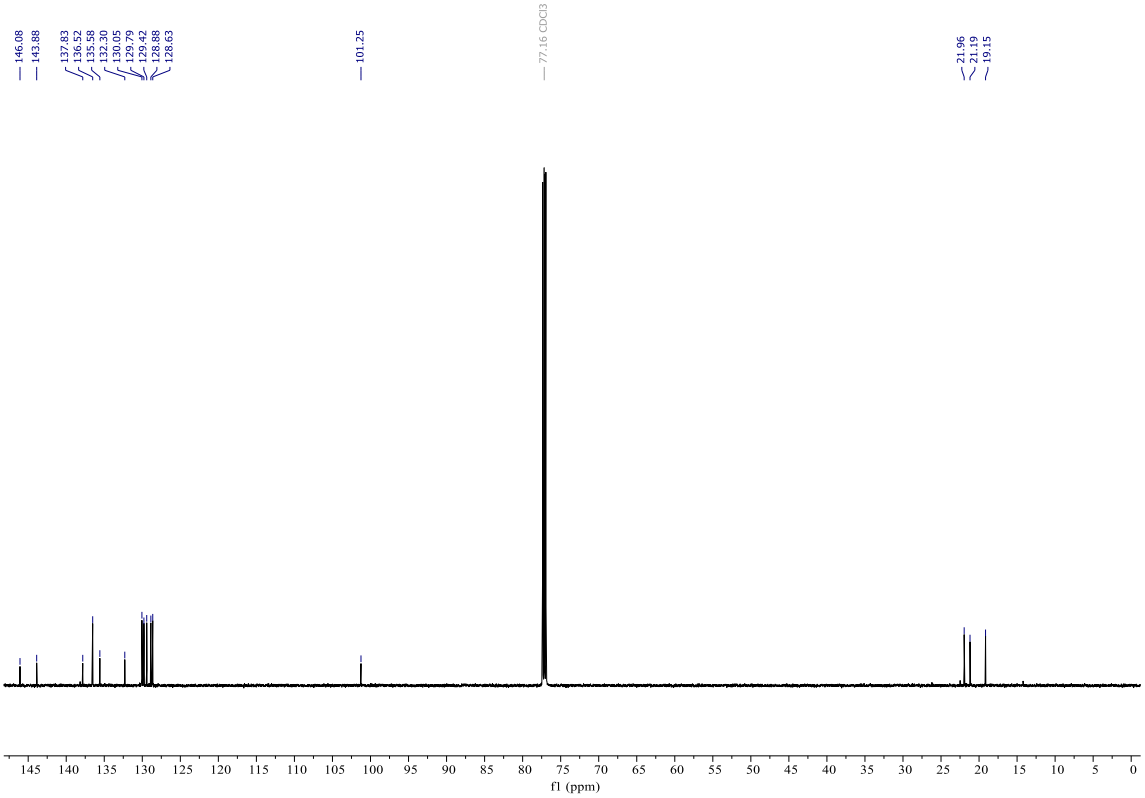
^{1}H-NMR spectrum of **18**. 300 MHz, $CDCl_3$



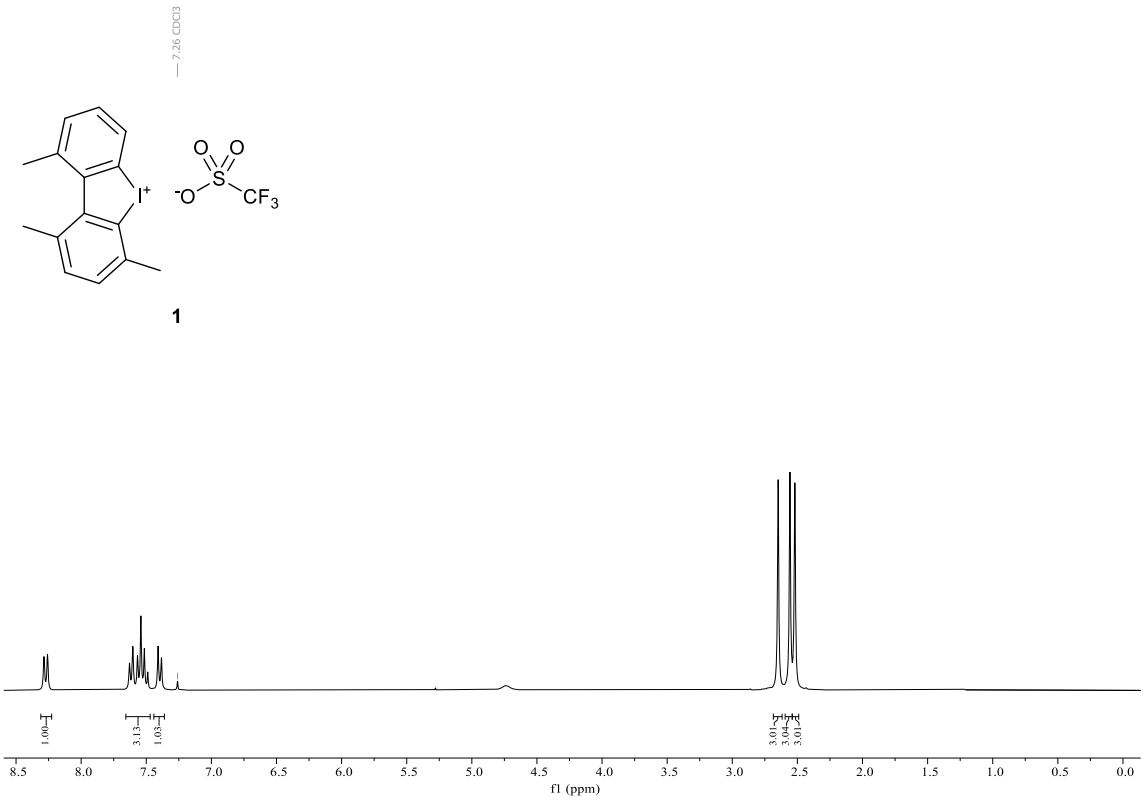
^{13}C-NMR spectrum of **18**. 75.5 MHz, $CDCl_3$



^{1}H-NMR spectrum of **19**. 600 MHz, $CDCl_3$

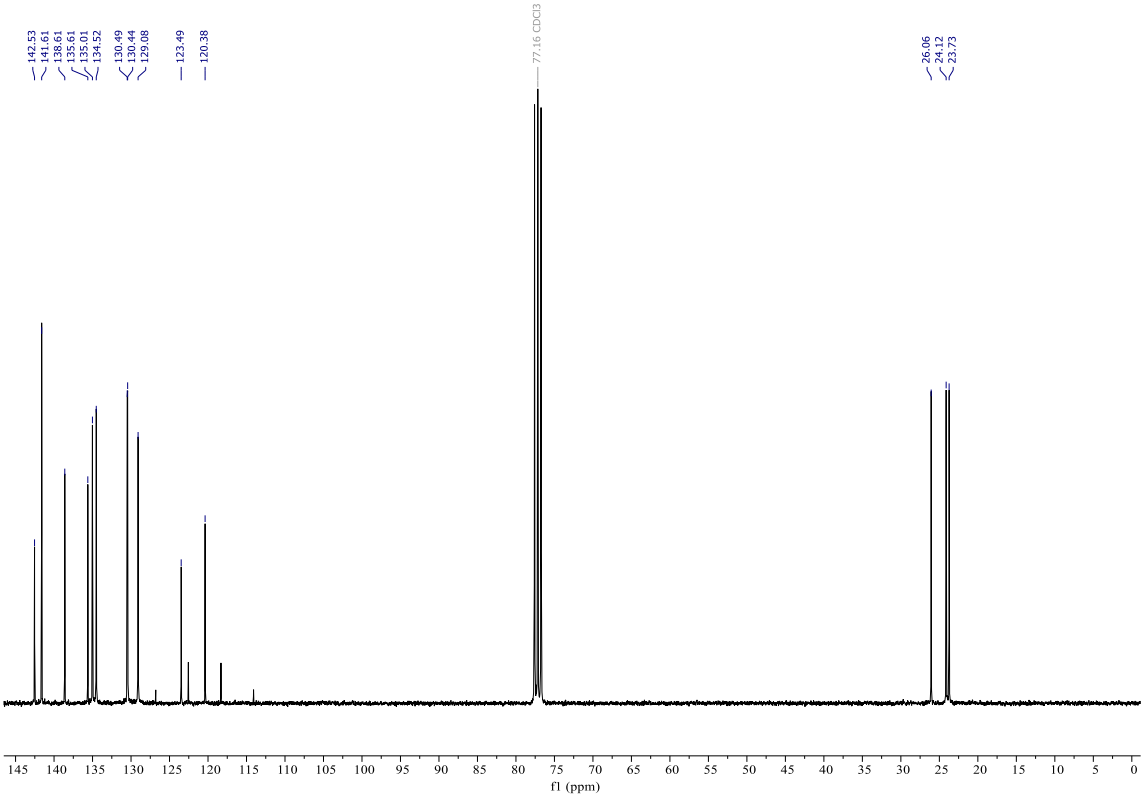


^{13}C-NMR spectrum of **19**. 151 MHz, $CDCl_3$

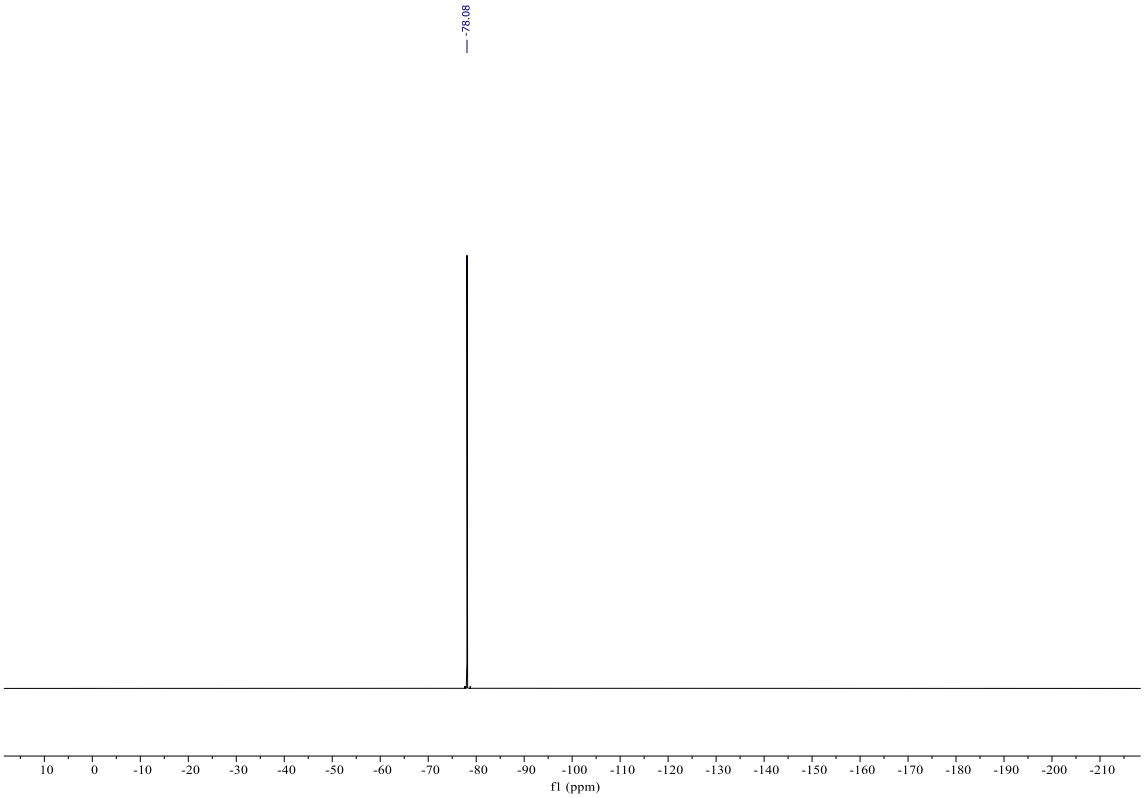


1

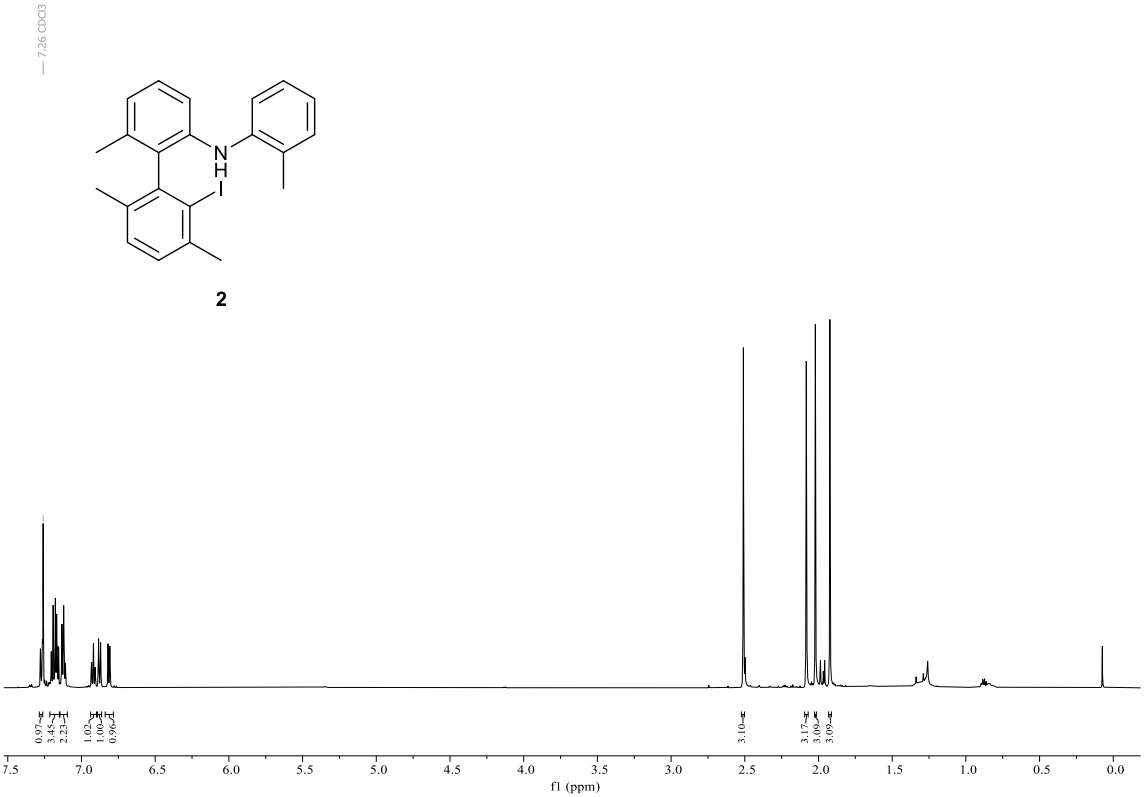
^{1}H-NMR spectrum of **1**. 300 MHz, $CDCl_3$



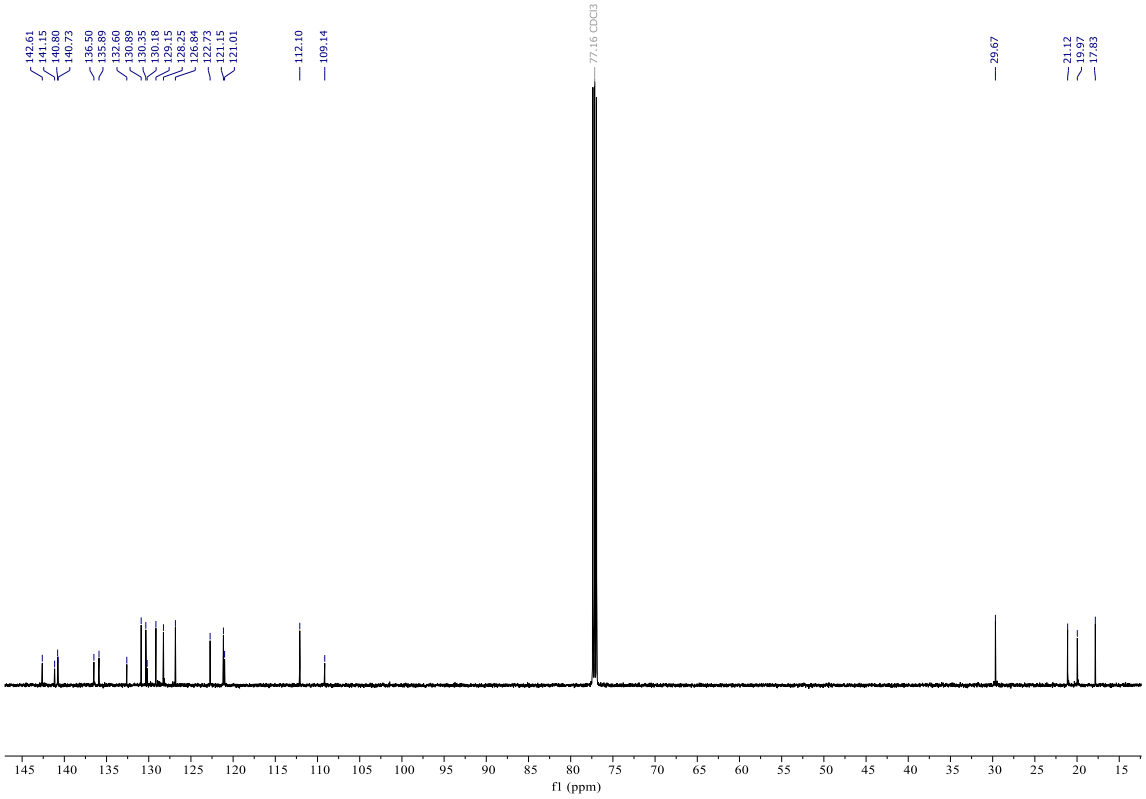
^{13}C-NMR spectrum of **1**. 75.5 MHz, $CDCl_3$



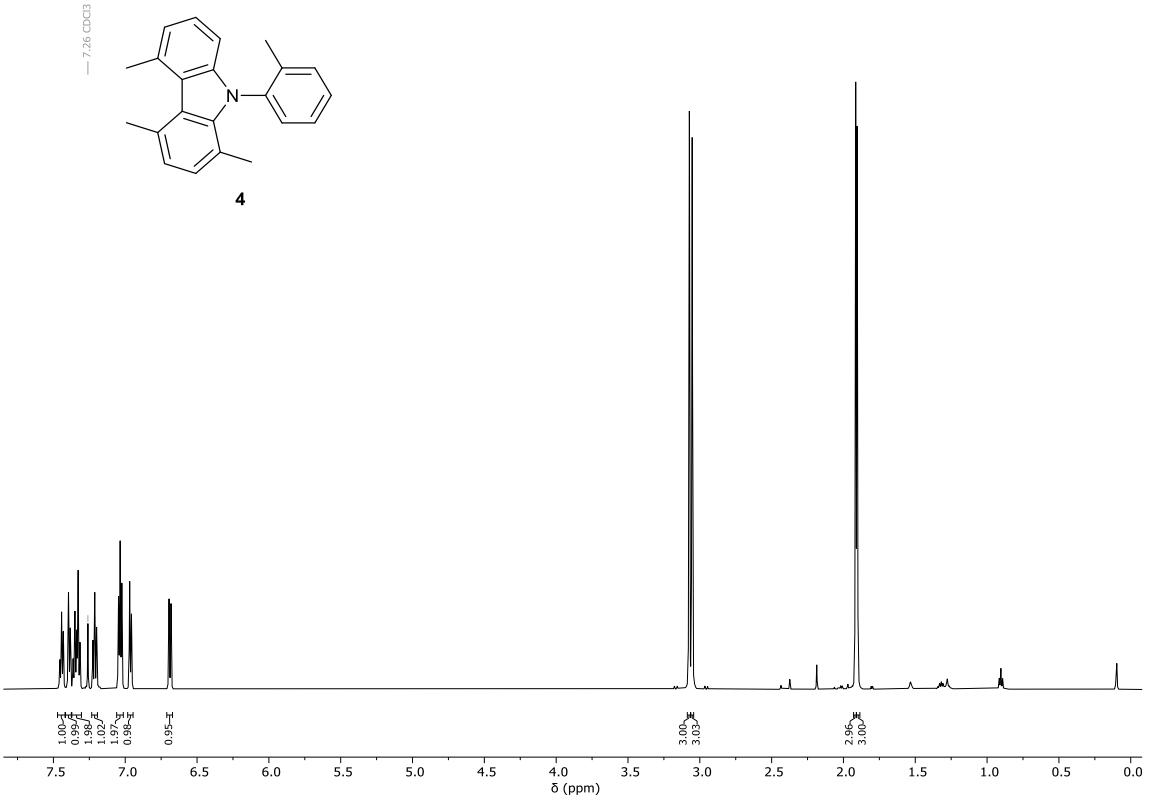
^{19}F-NMR spectrum of **1**. 282 MHz, $CDCl_3$



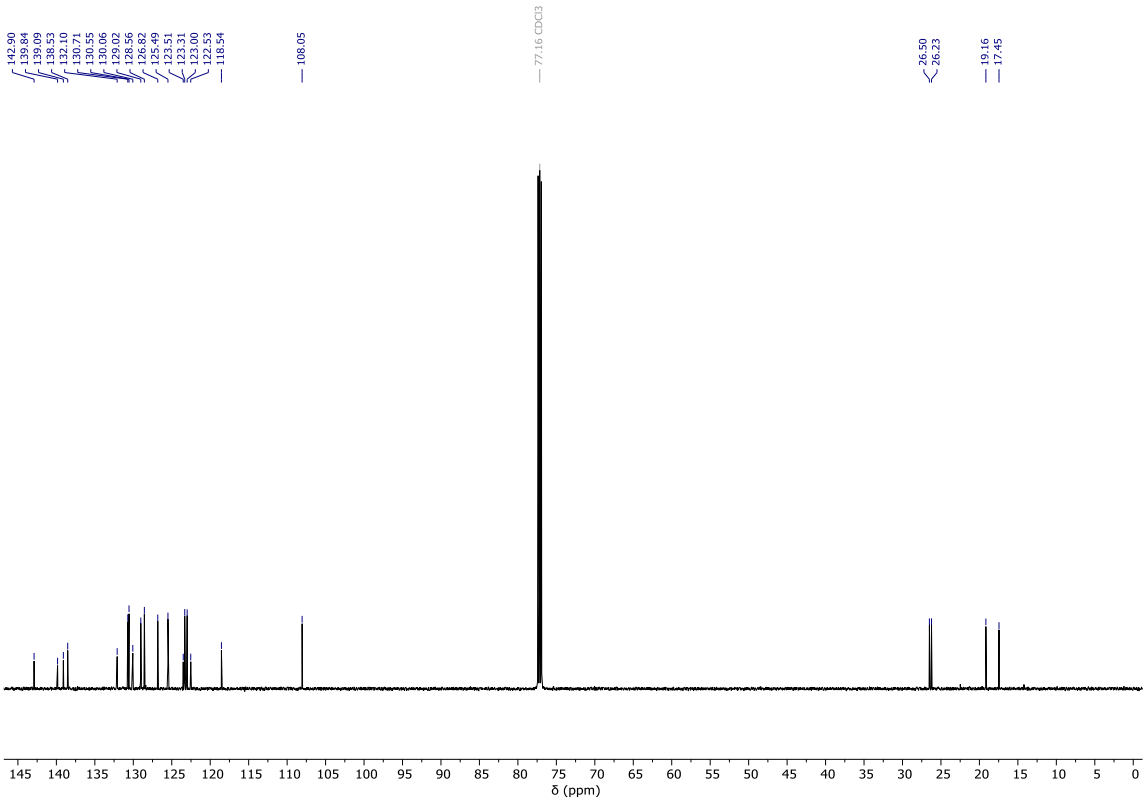
^{1}H-NMR spectrum of **2**. 600 MHz, $CDCl_3$



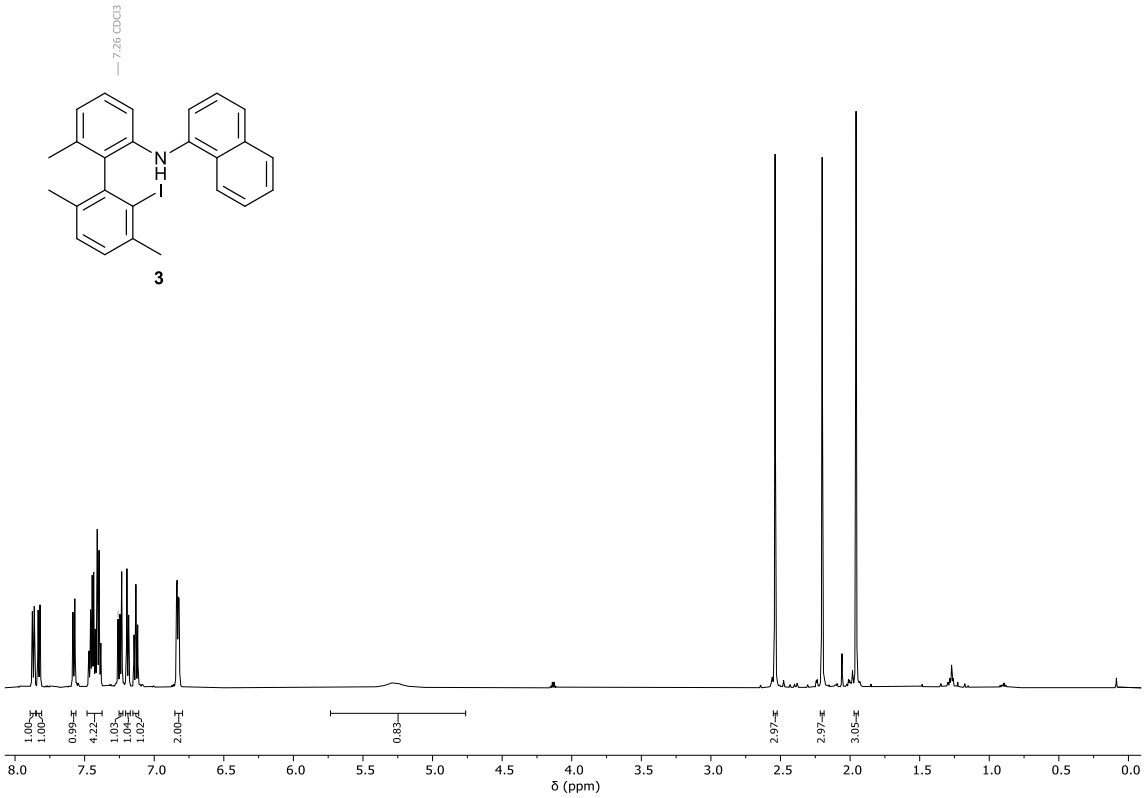
^{13}C-NMR spectrum of **2**. 151 MHz, $CDCl_3$



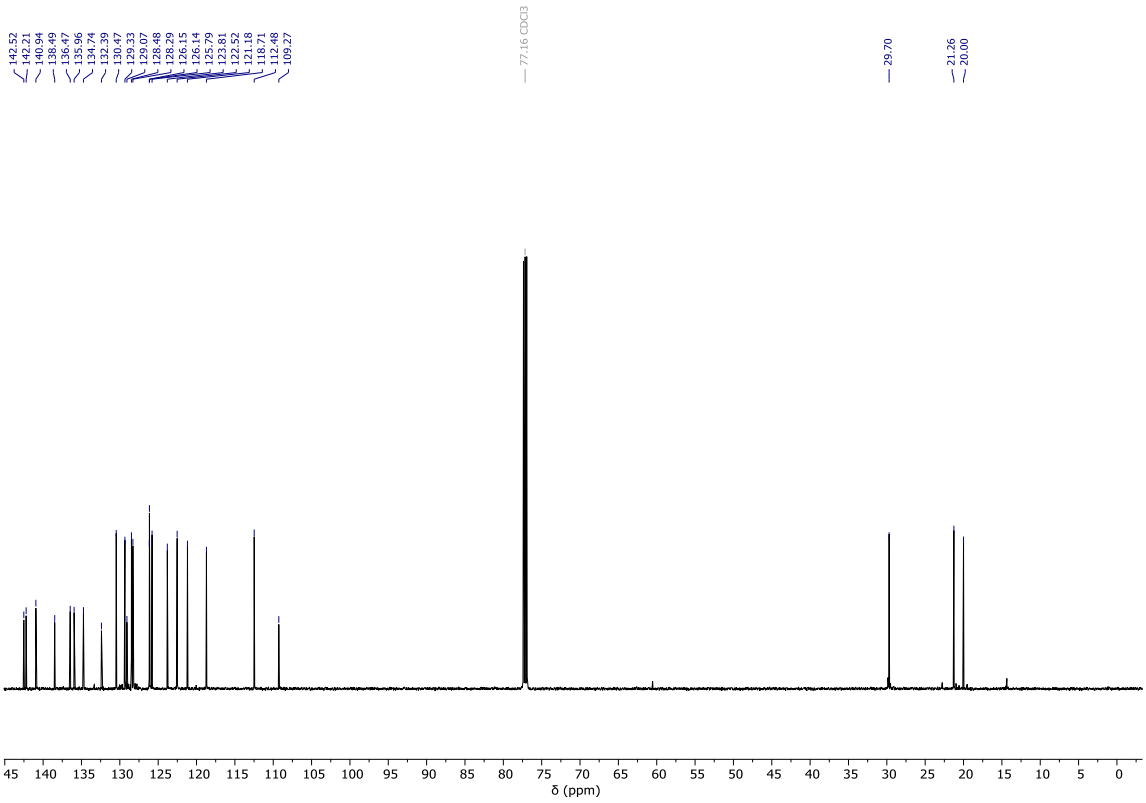
^{1}H-NMR spectrum of **4**. 600 MHz, $CDCl_3$



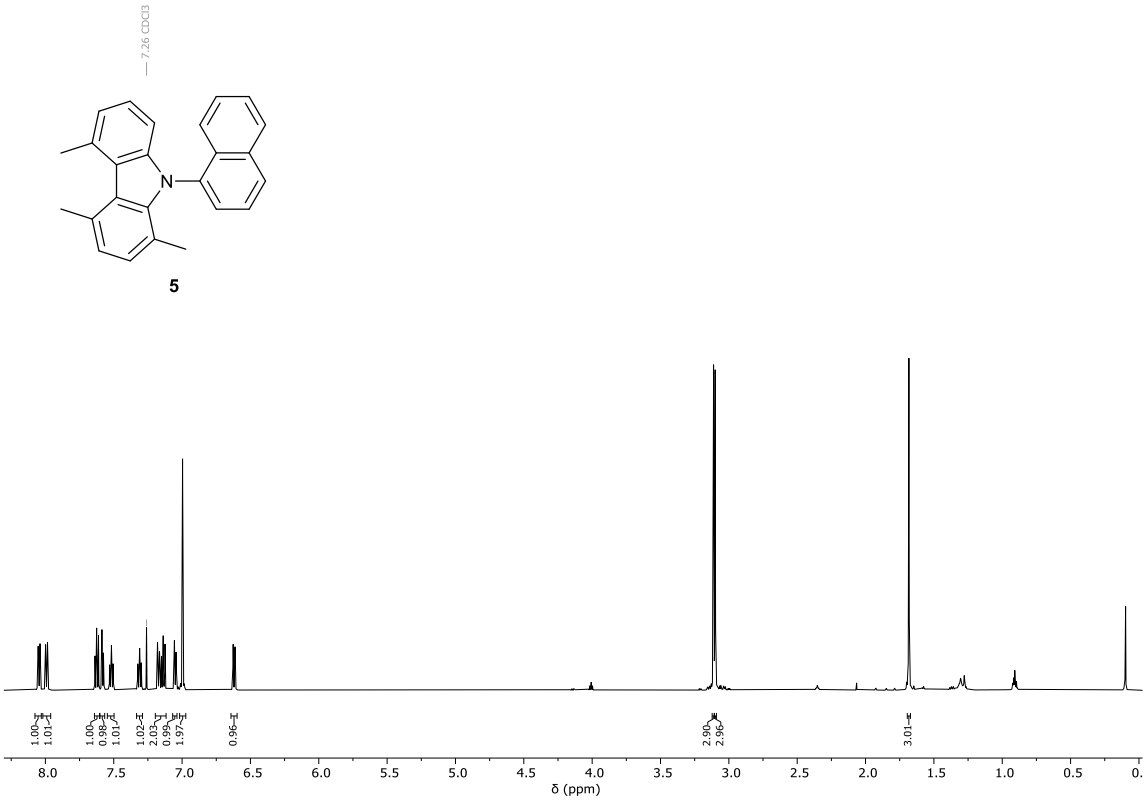
^{13}C-NMR spectrum of **4**. 151 MHz, $CDCl_3$



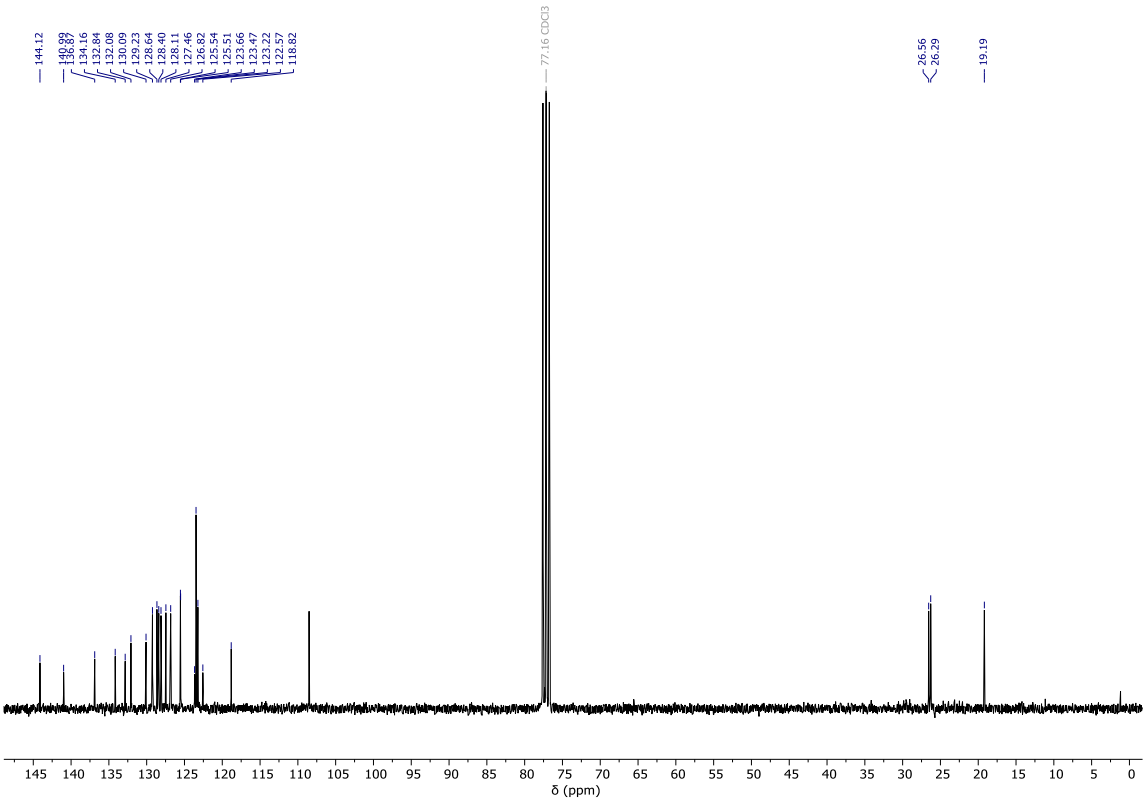
^{1}H-NMR spectrum of **3**. 600 MHz, $CDCl_3$



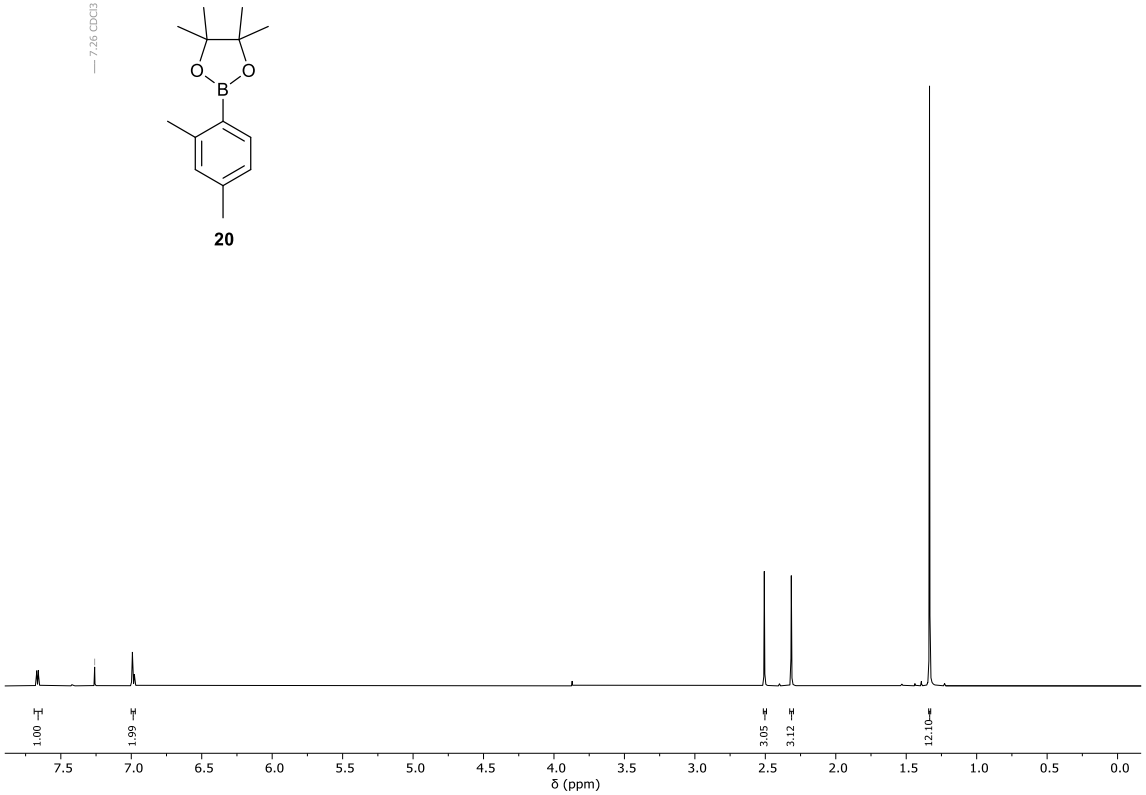
^{13}C-NMR spectrum of **3**. 75.5 MHz, $CDCl_3$



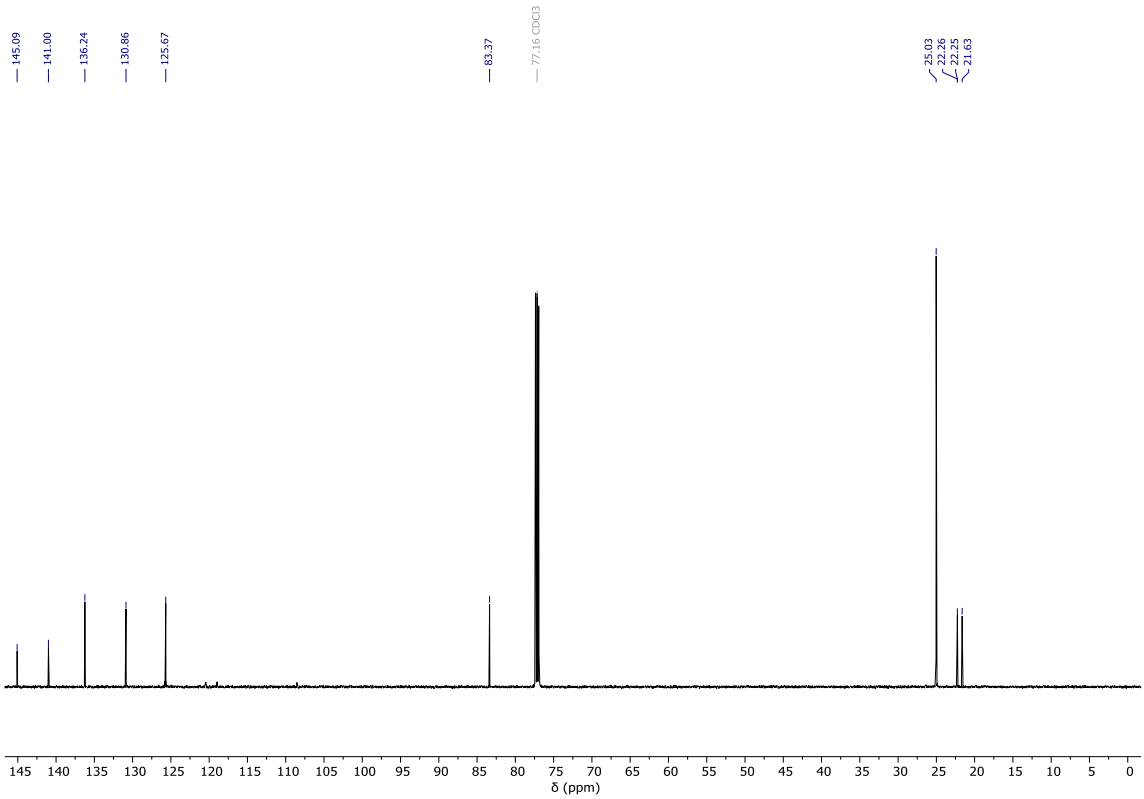
^{1}H-NMR spectrum of **5**. 600 MHz, $CDCl_3$



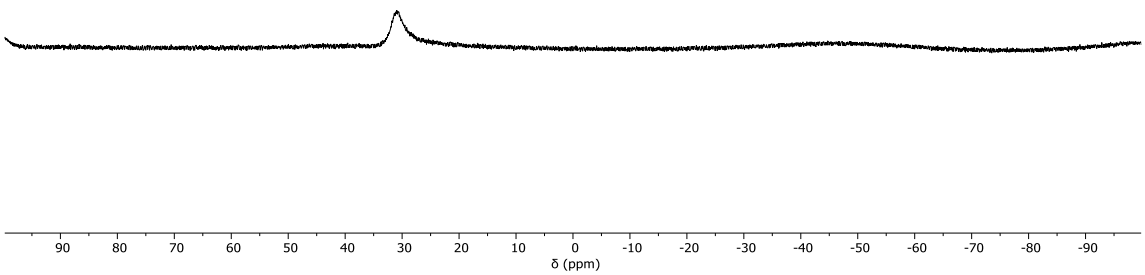
^{13}C-NMR spectrum of **5**. 75.5 MHz, $CDCl_3$



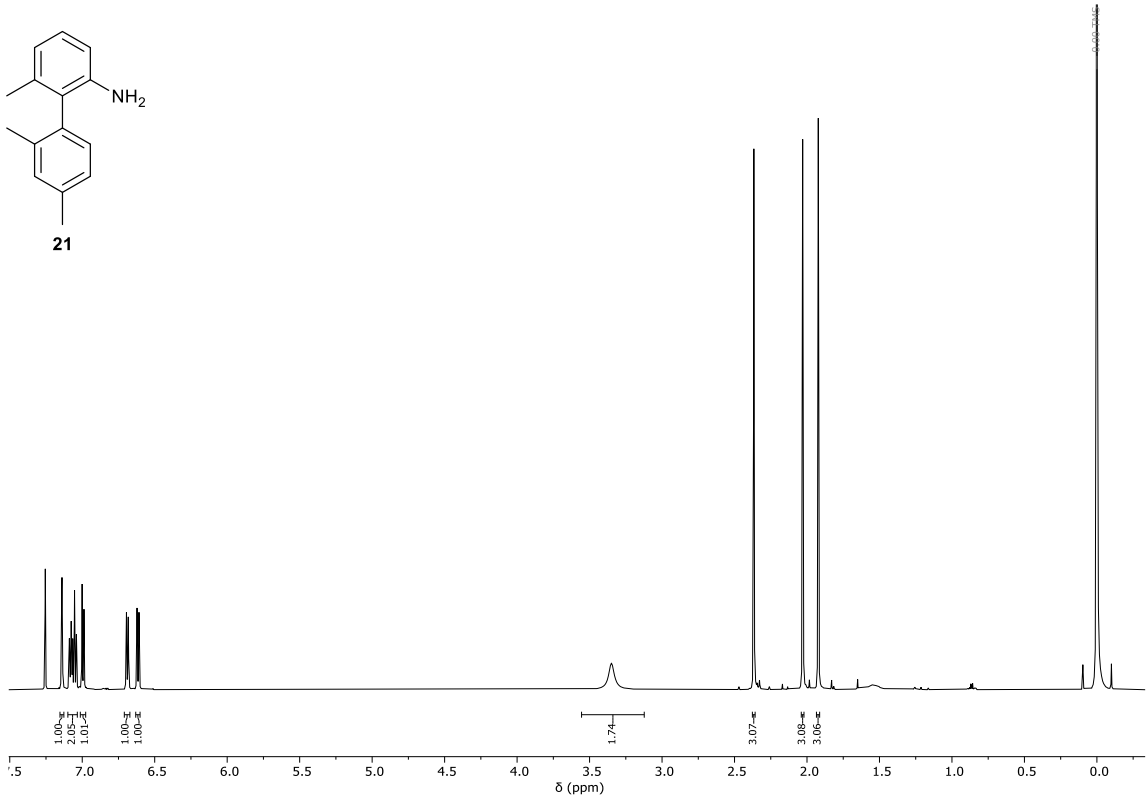
^{1}H-NMR spectrum of **20**. 600 MHz, $CDCl_3$



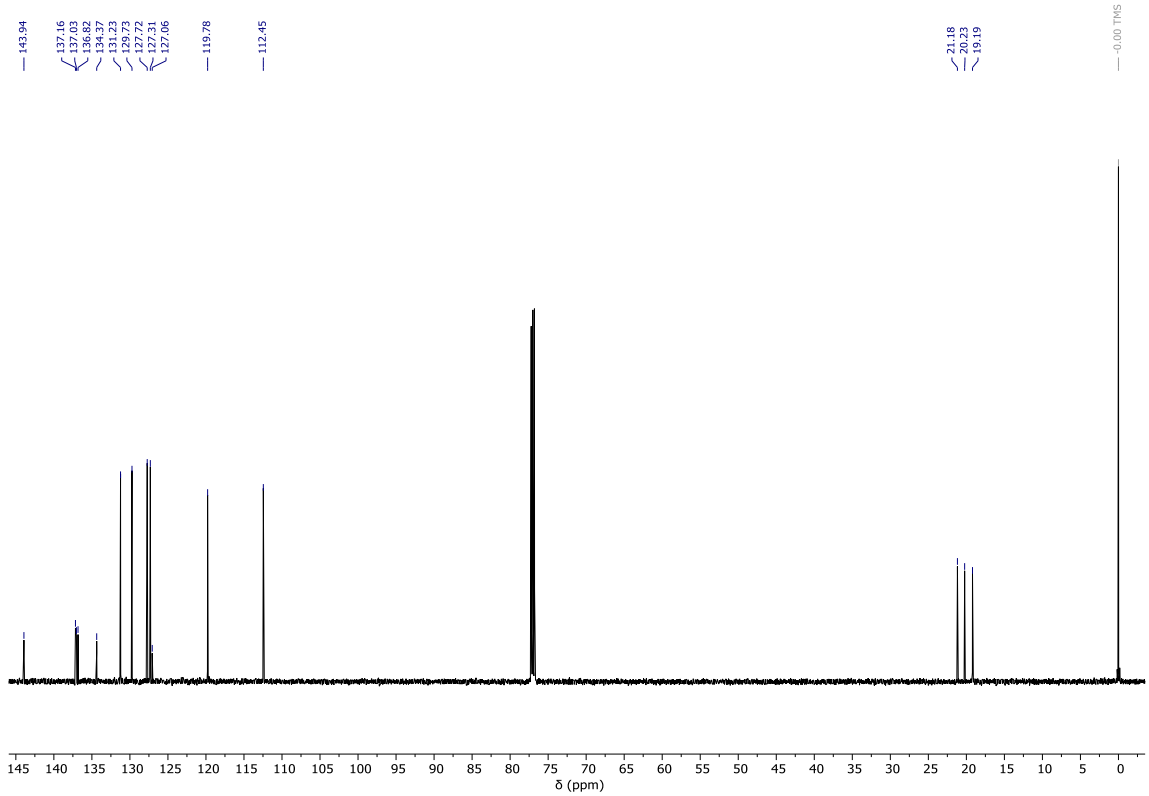
^{13}C-NMR spectrum of **20**. 151 MHz, $CDCl_3$



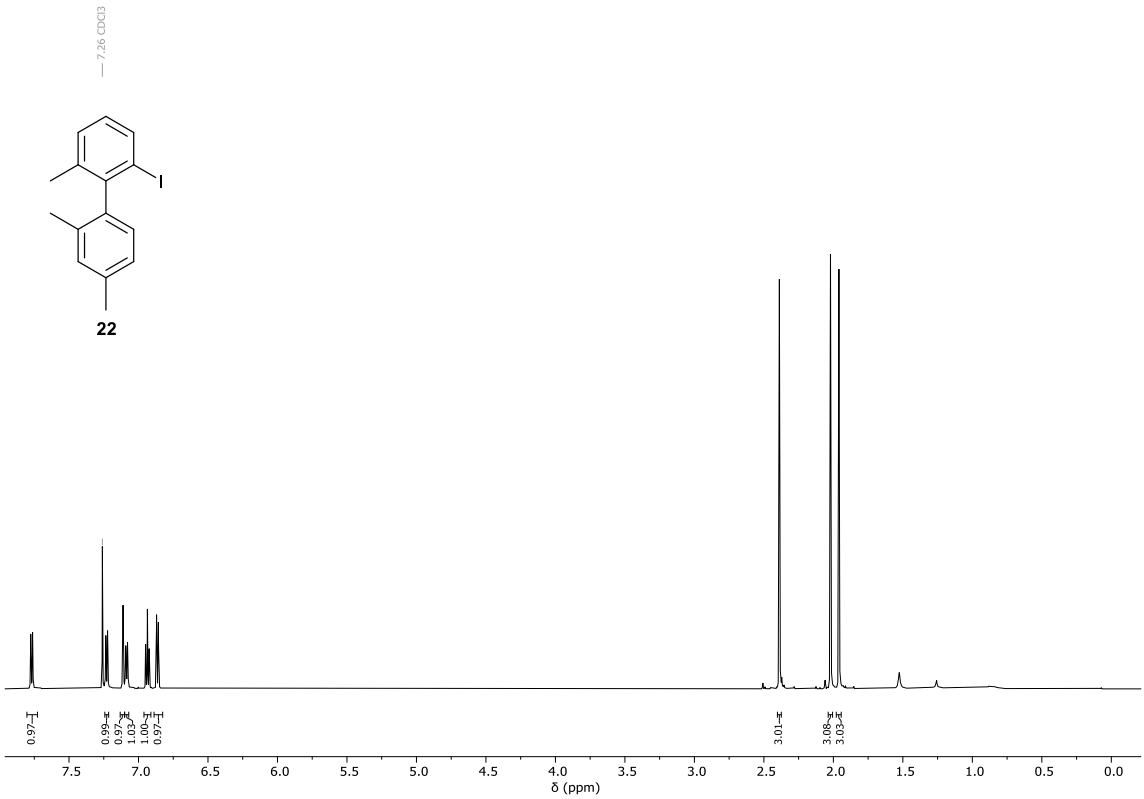
^{11}B-NMR spectrum of **20**. 96 MHz, $CDCl_3$



^{1}H-NMR spectrum of **21**. 600 MHz, $CDCl_3$



^{13}C-NMR spectrum of **21**. 151 MHz, $CDCl_3$



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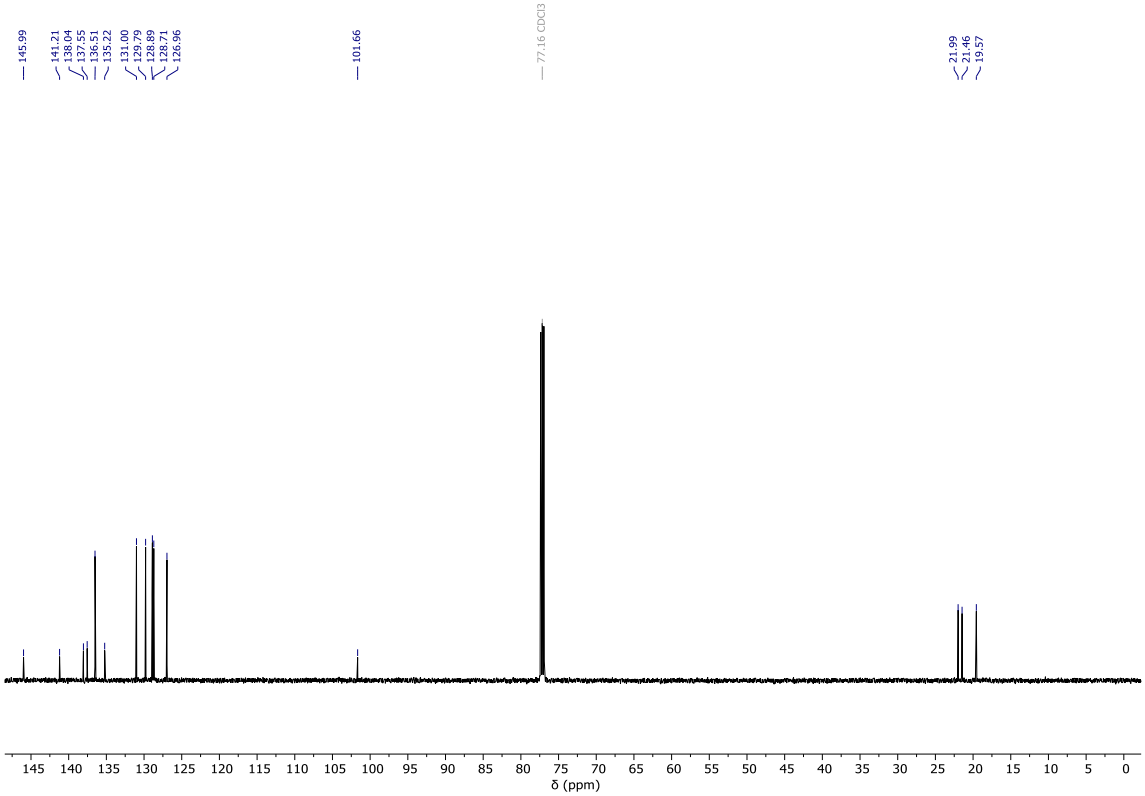

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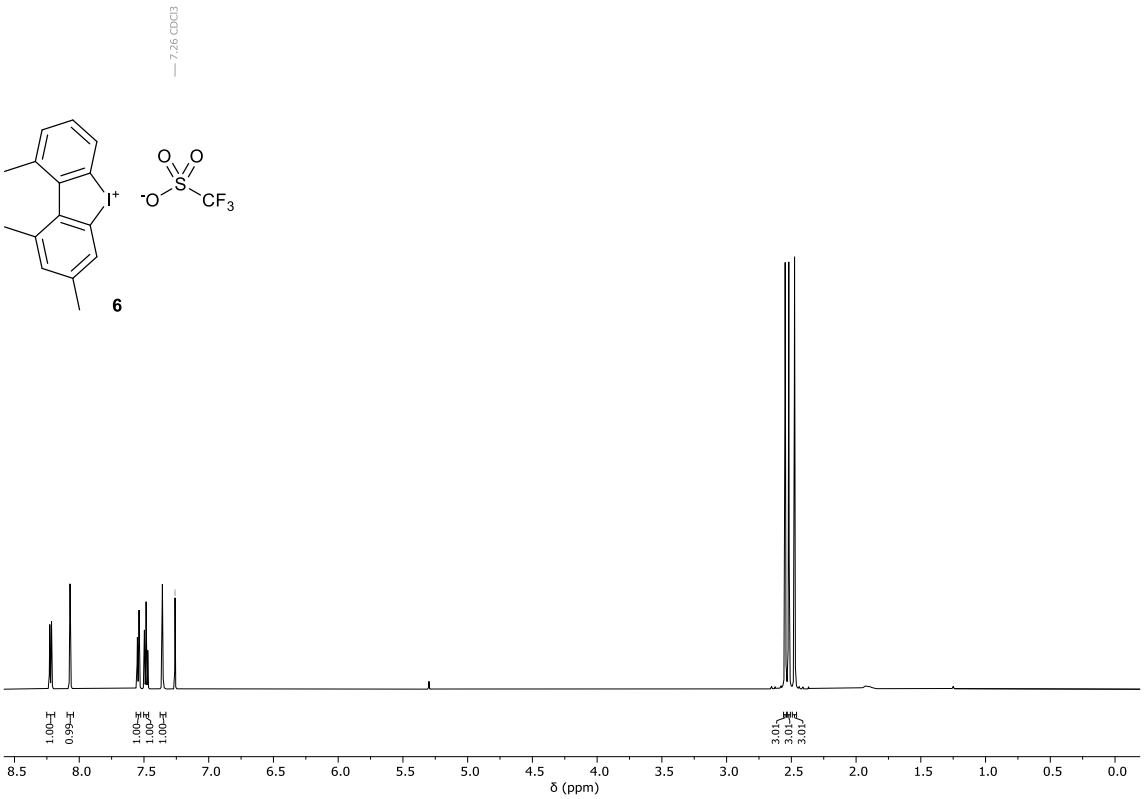
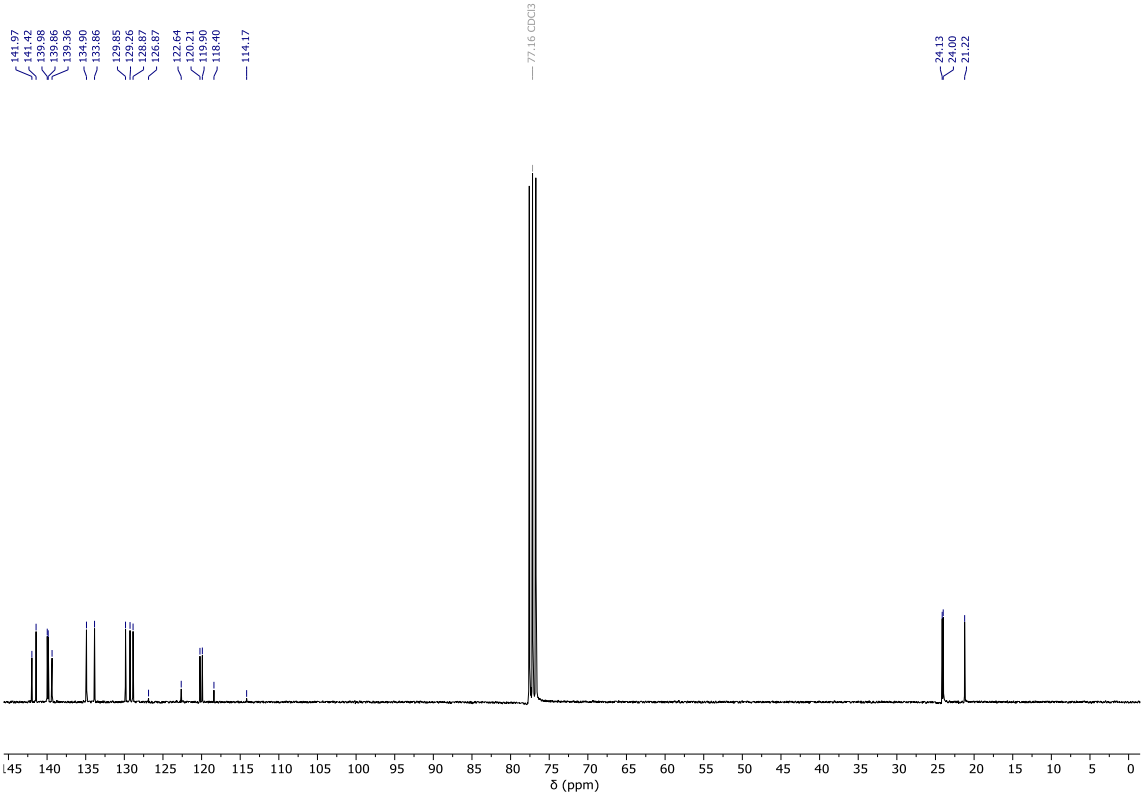
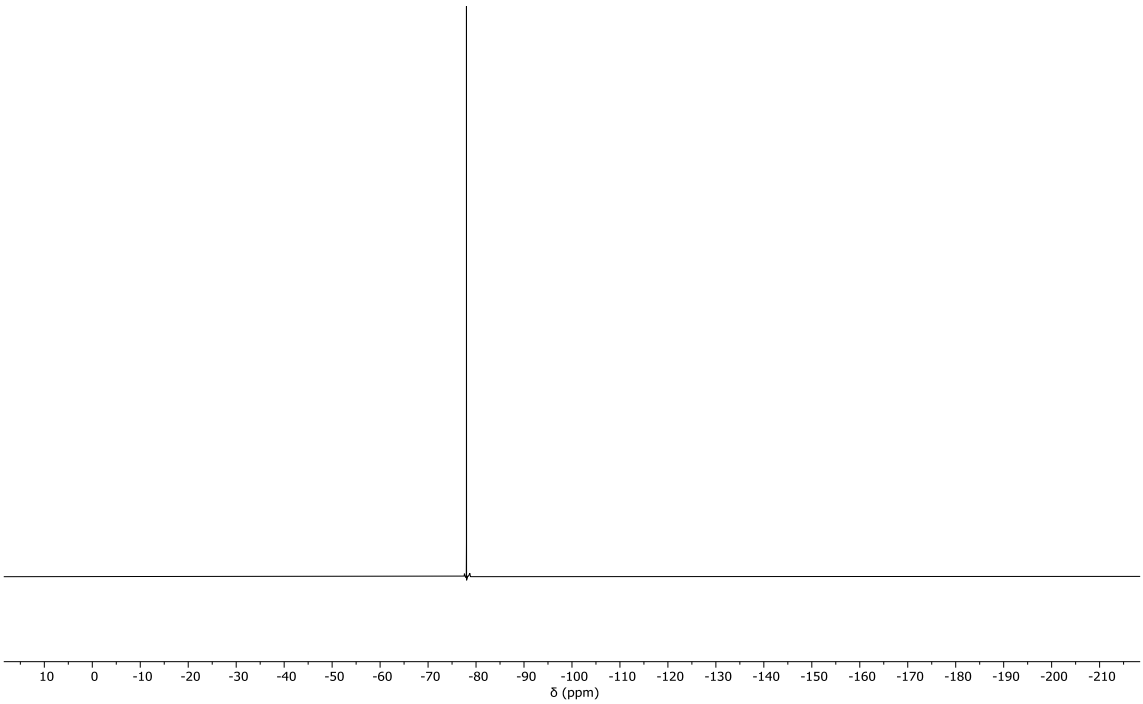


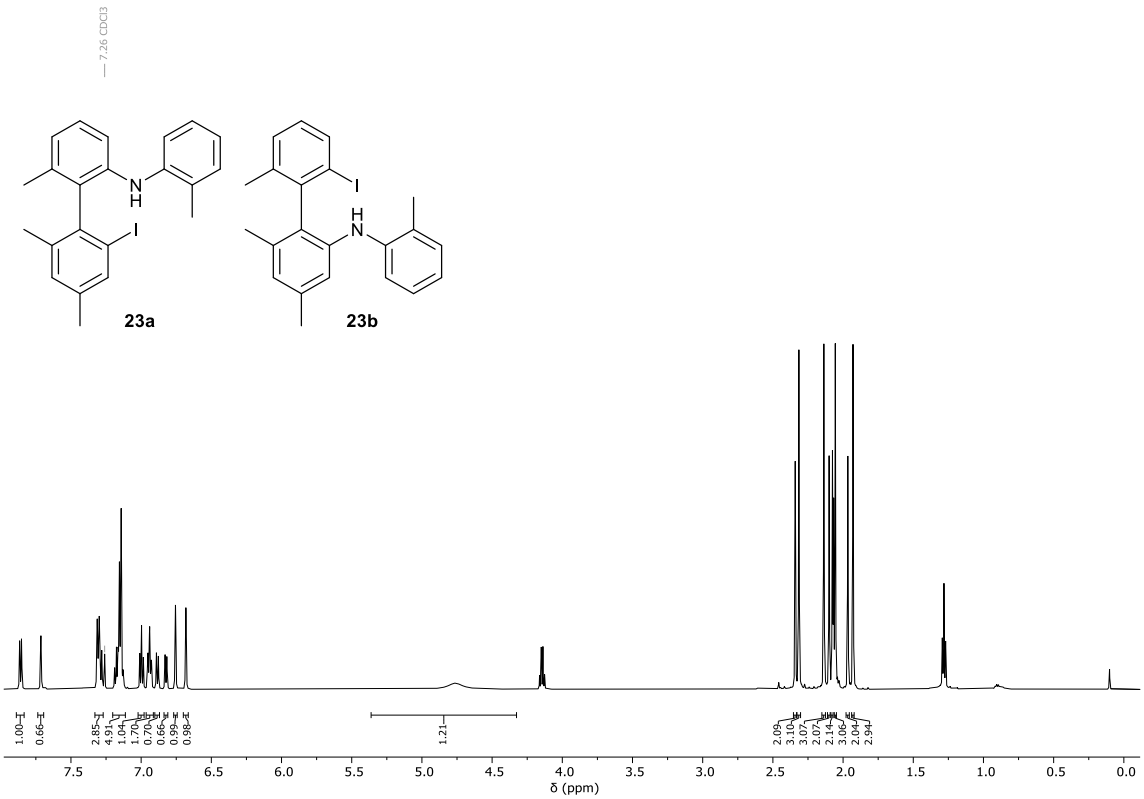
^{1}H-NMR spectrum of **6**. 600 MHz, $CDCl_3$



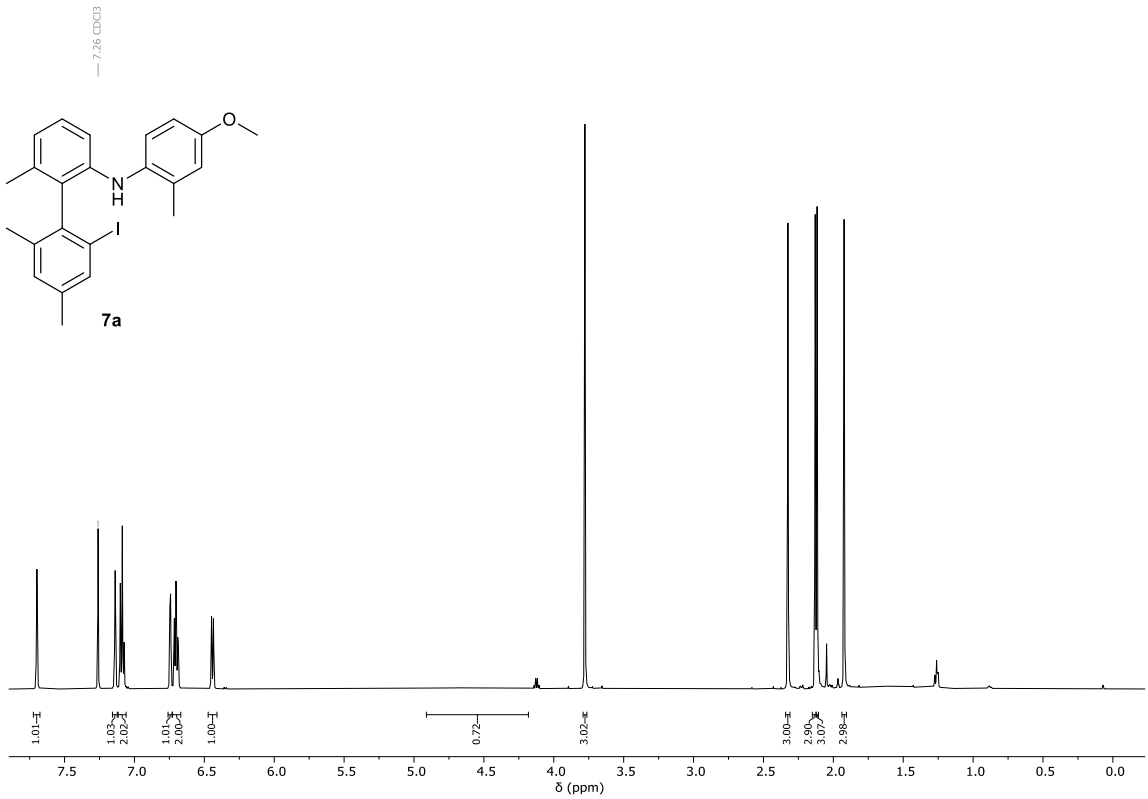
^{13}C-NMR spectrum of **6**. 151 MHz, $CDCl_3$



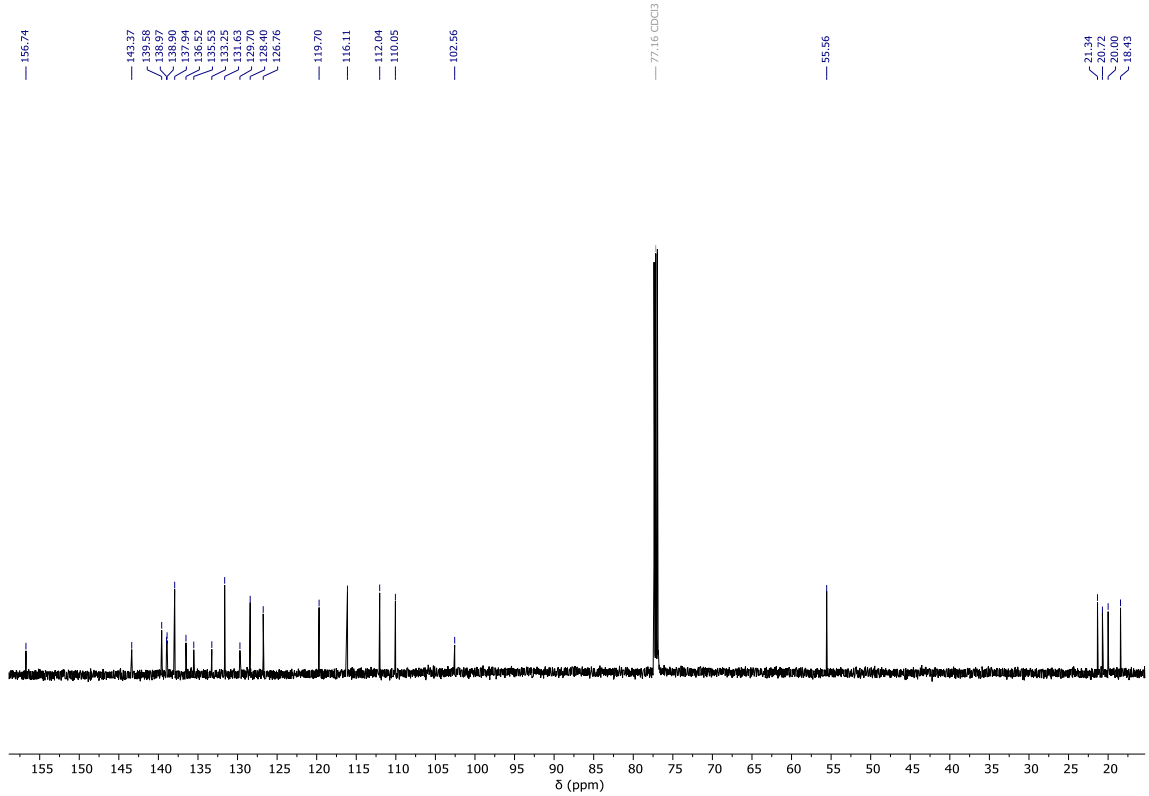
^{19}F-NMR spectrum of **6**. 282 MHz, $CDCl_3$



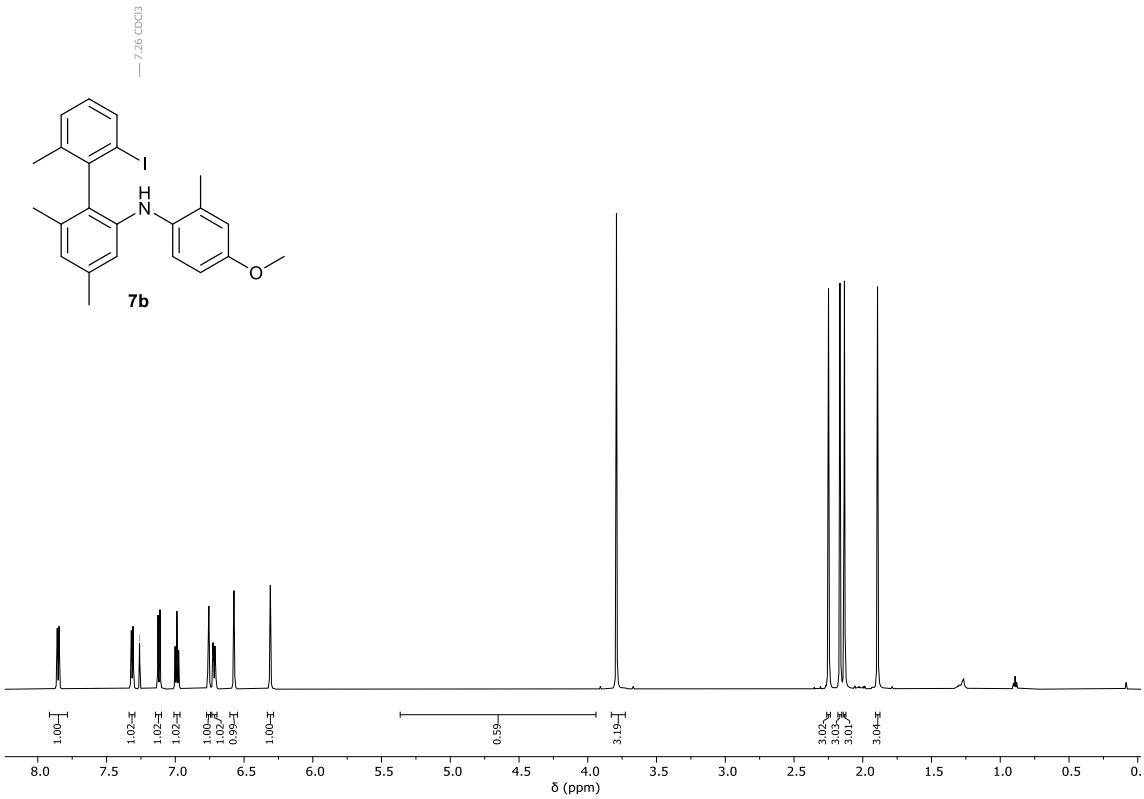
^{1}H-NMR spectrum of **23a** & **23b**. 600 MHz, $CDCl_3$



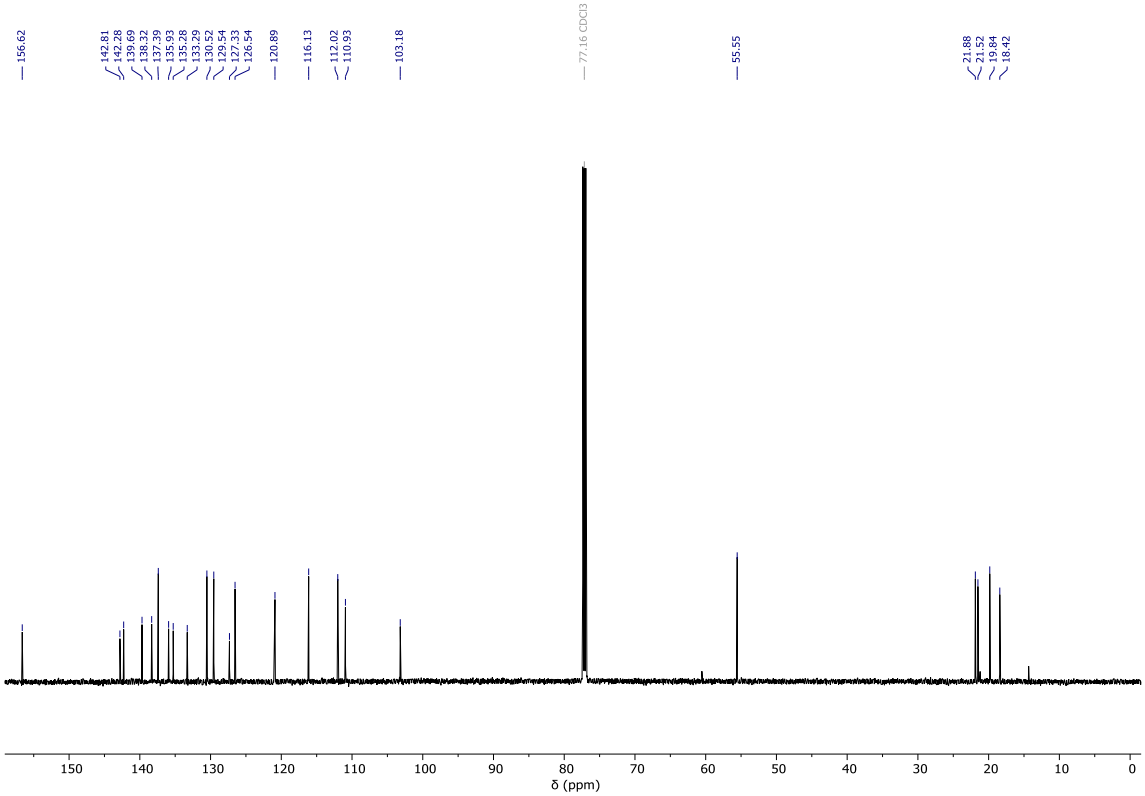
^{1}H-NMR spectrum of **7a**. 600 MHz, $CDCl_3$



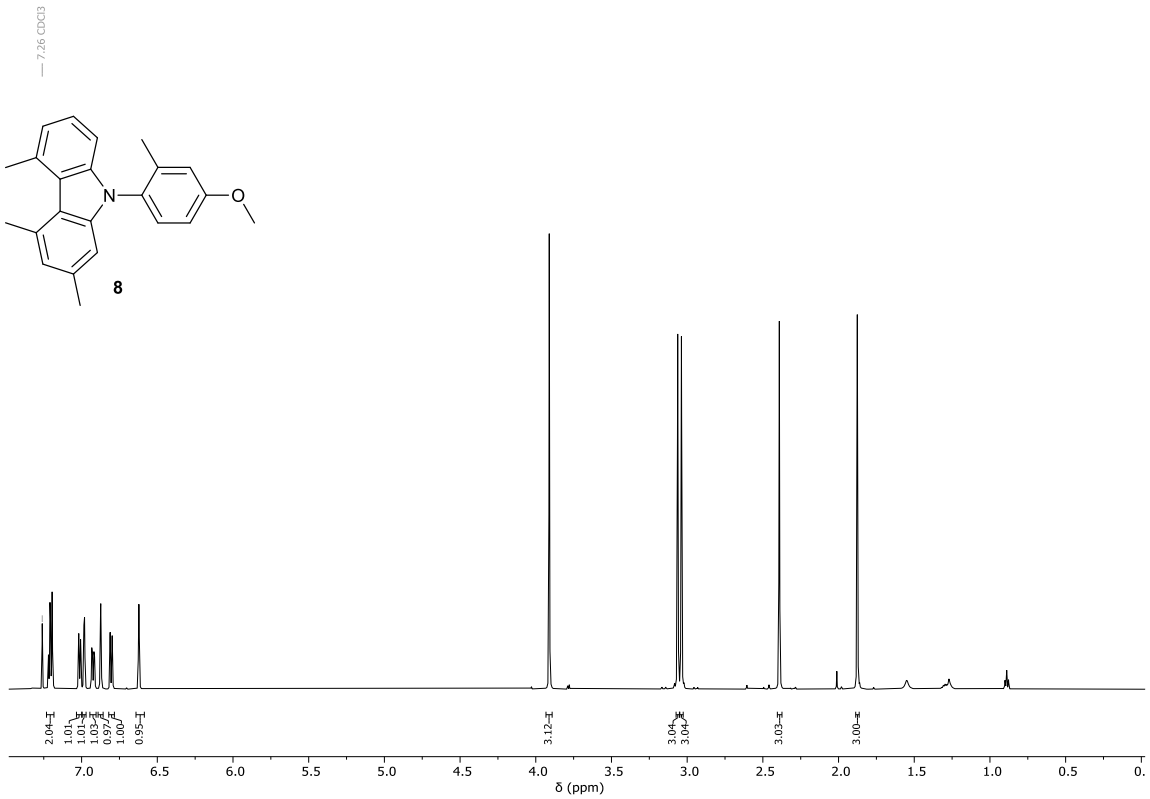
^{13}C-NMR spectrum of **7a**. 151 MHz, $CDCl_3$



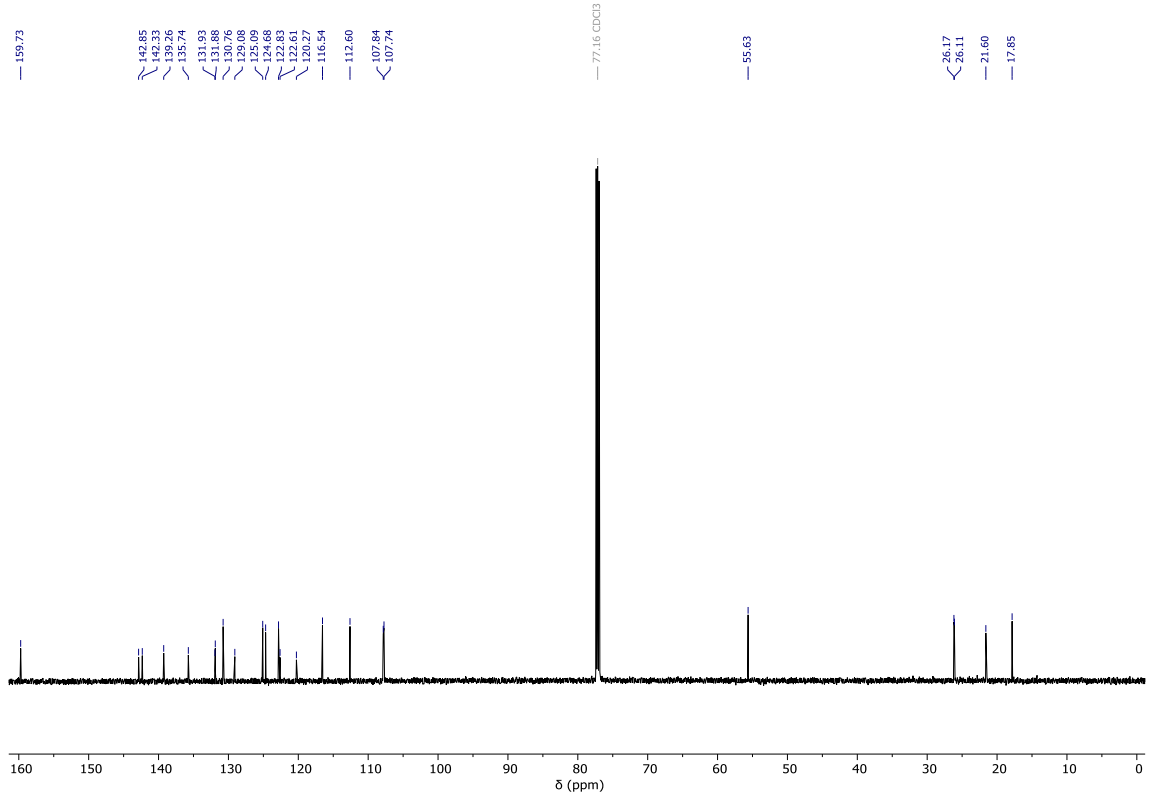
^{1}H-NMR spectrum of **7b**. 600 MHz, $CDCl_3$



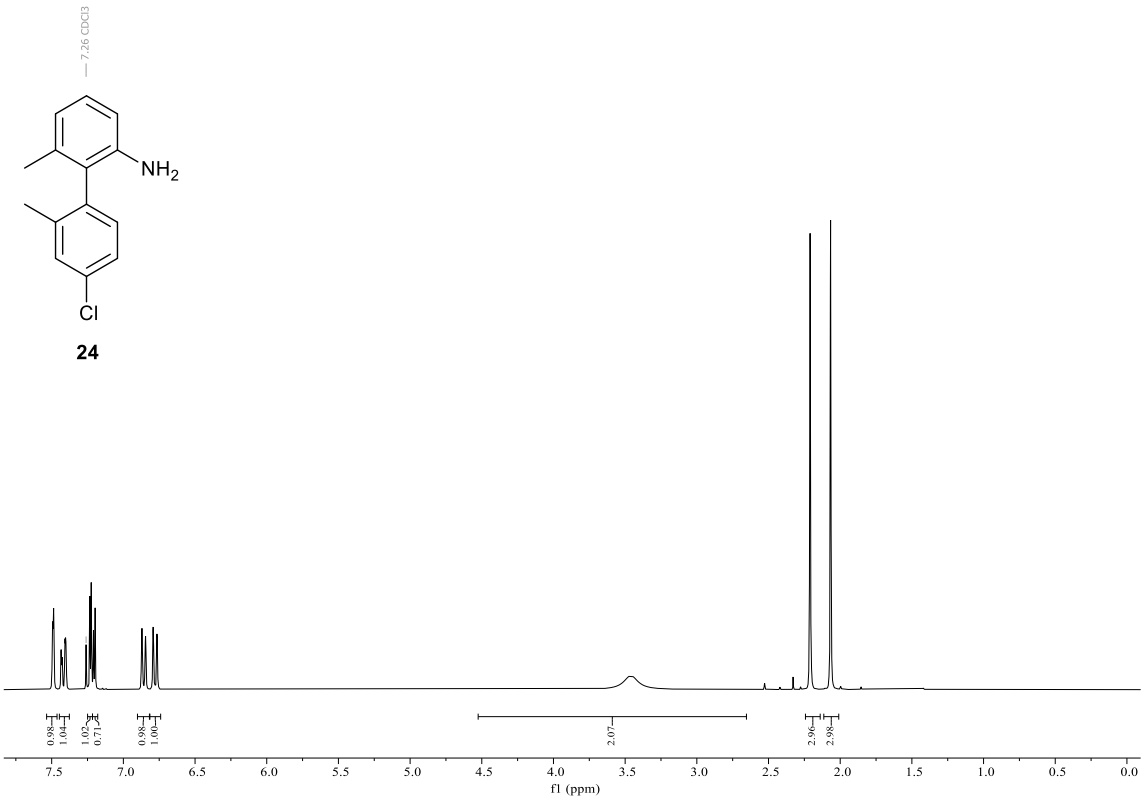
^{13}C-NMR spectrum of **7b**. 151 MHz, $CDCl_3$



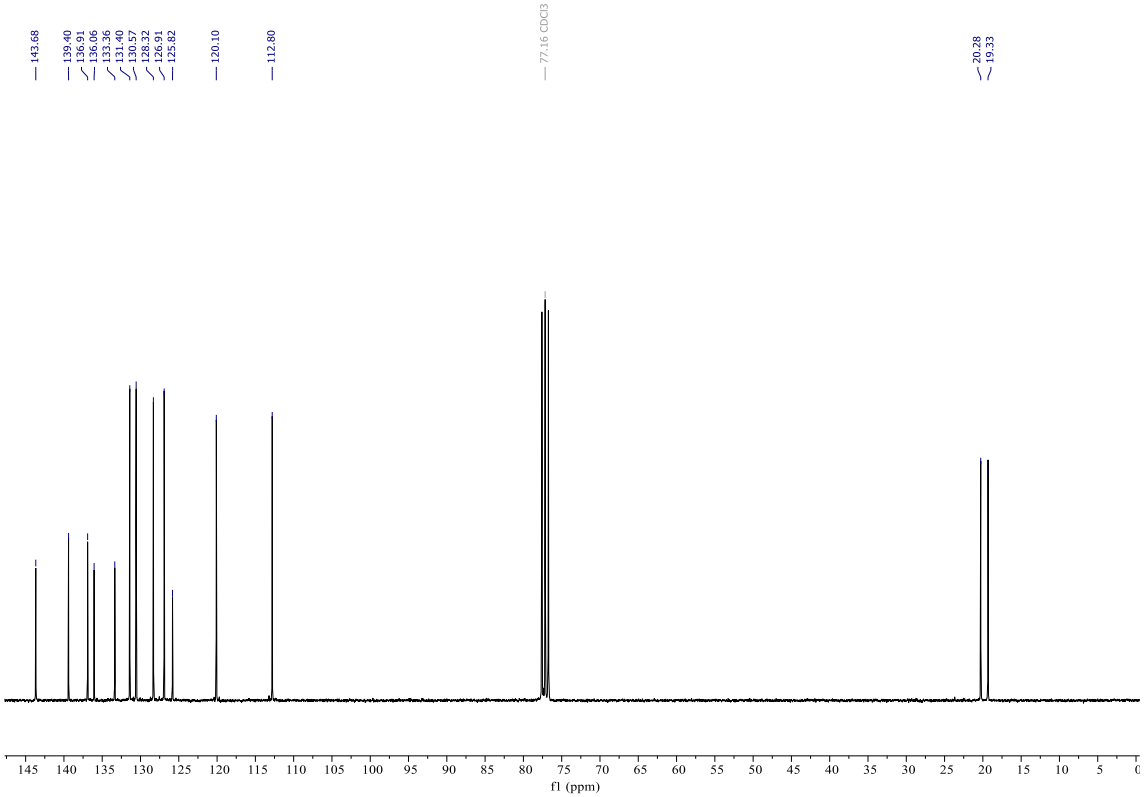
^{1}H-NMR spectrum of **8**. 600 MHz, $CDCl_3$



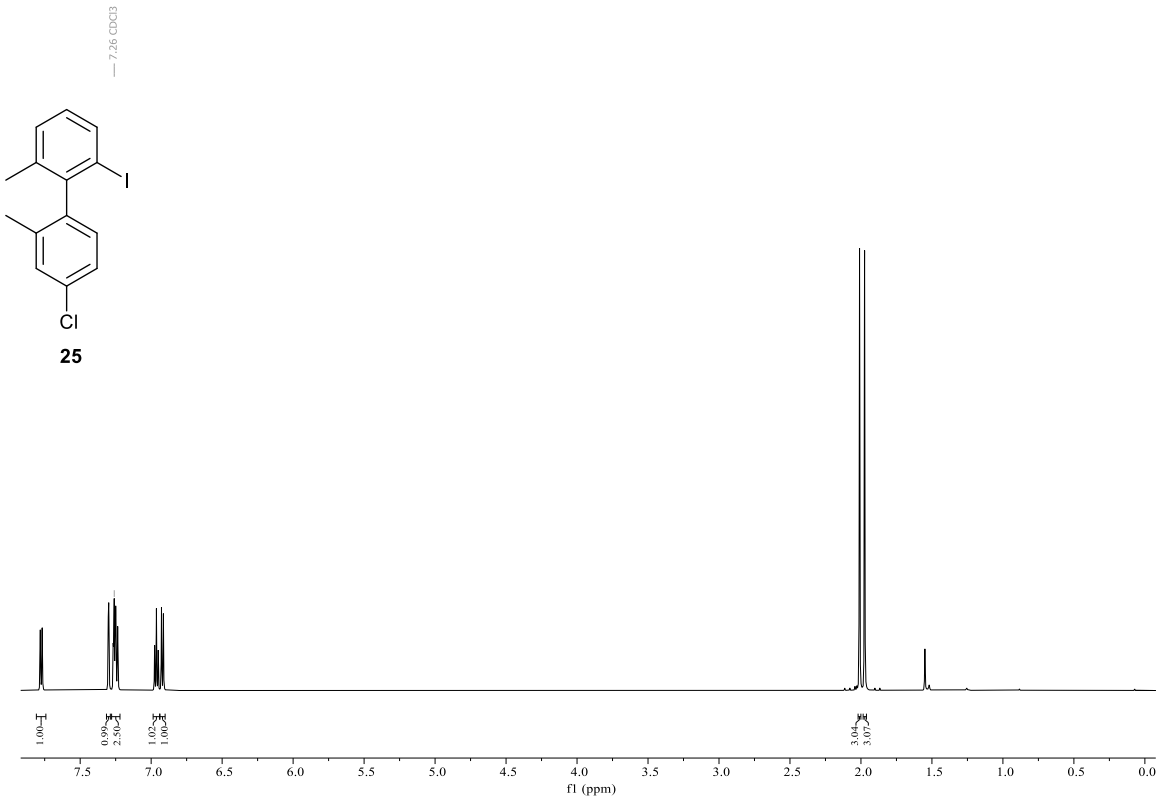
^{13}C-NMR spectrum of **8**. 151 MHz, $CDCl_3$



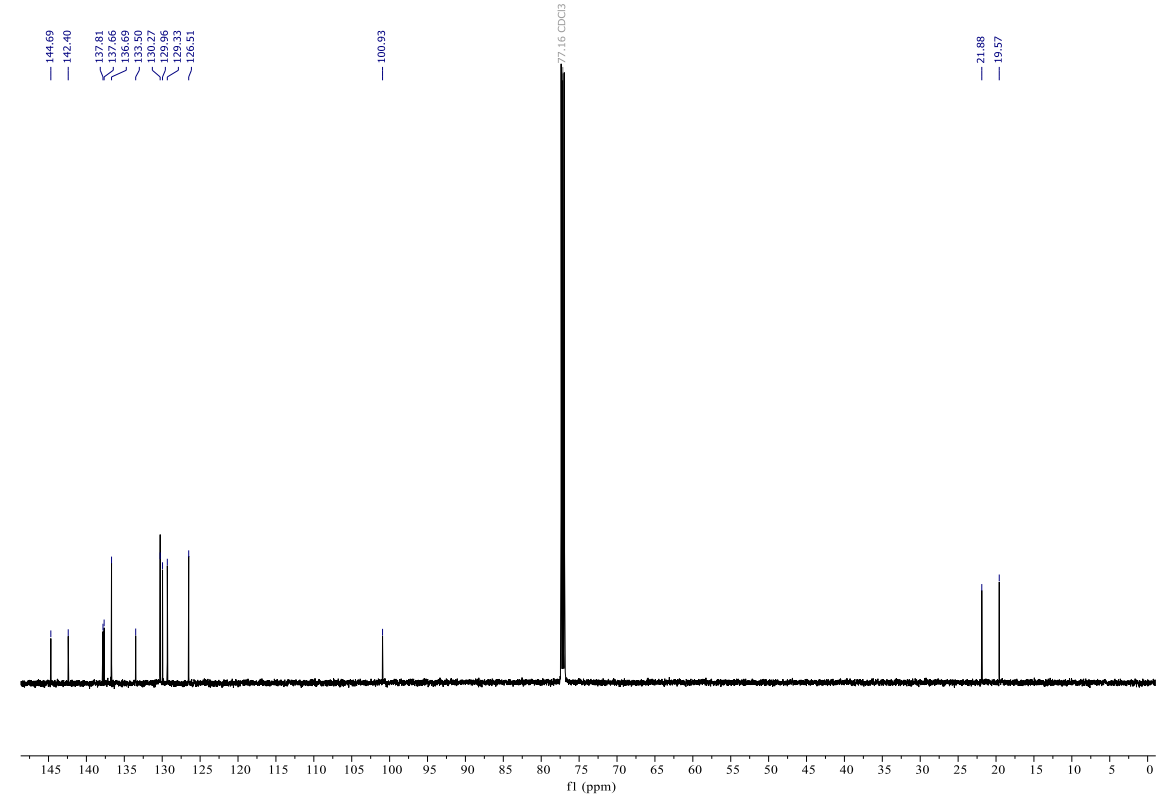
^{1}H-NMR spectrum of **24**. 300 MHz, $CDCl_3$



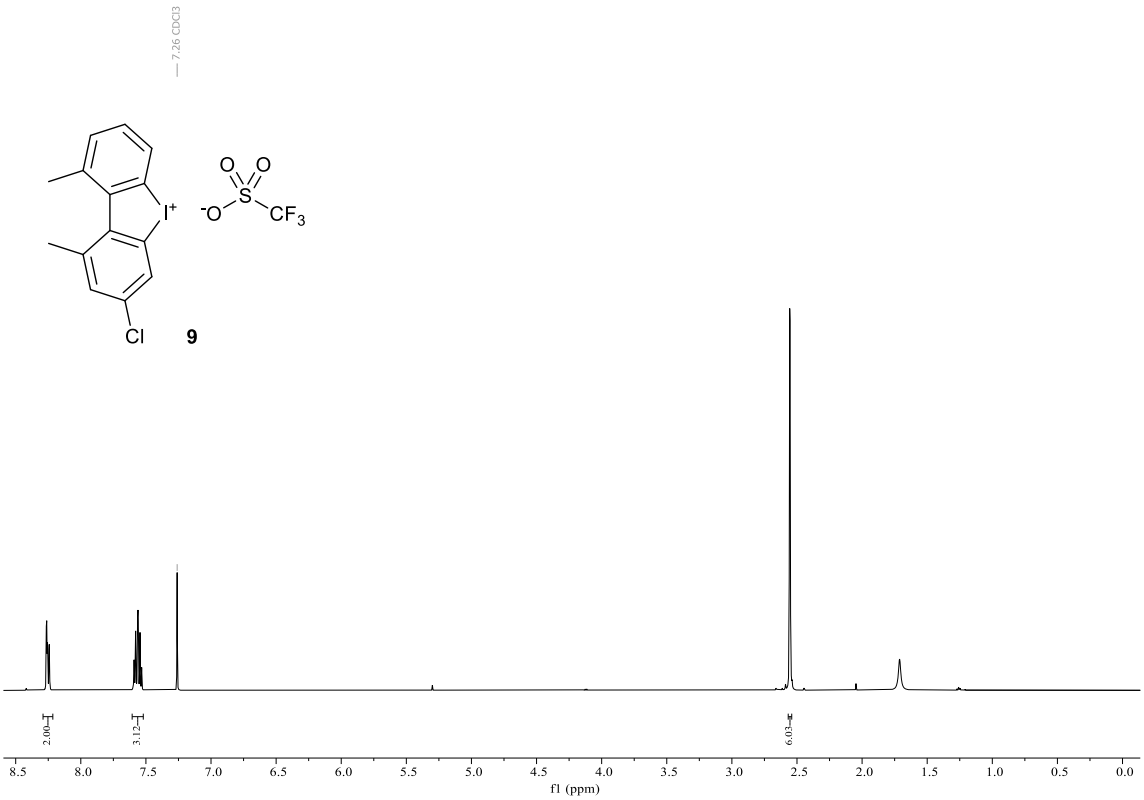
^{13}C-NMR spectrum of **24**. 75.5 MHz, $CDCl_3$



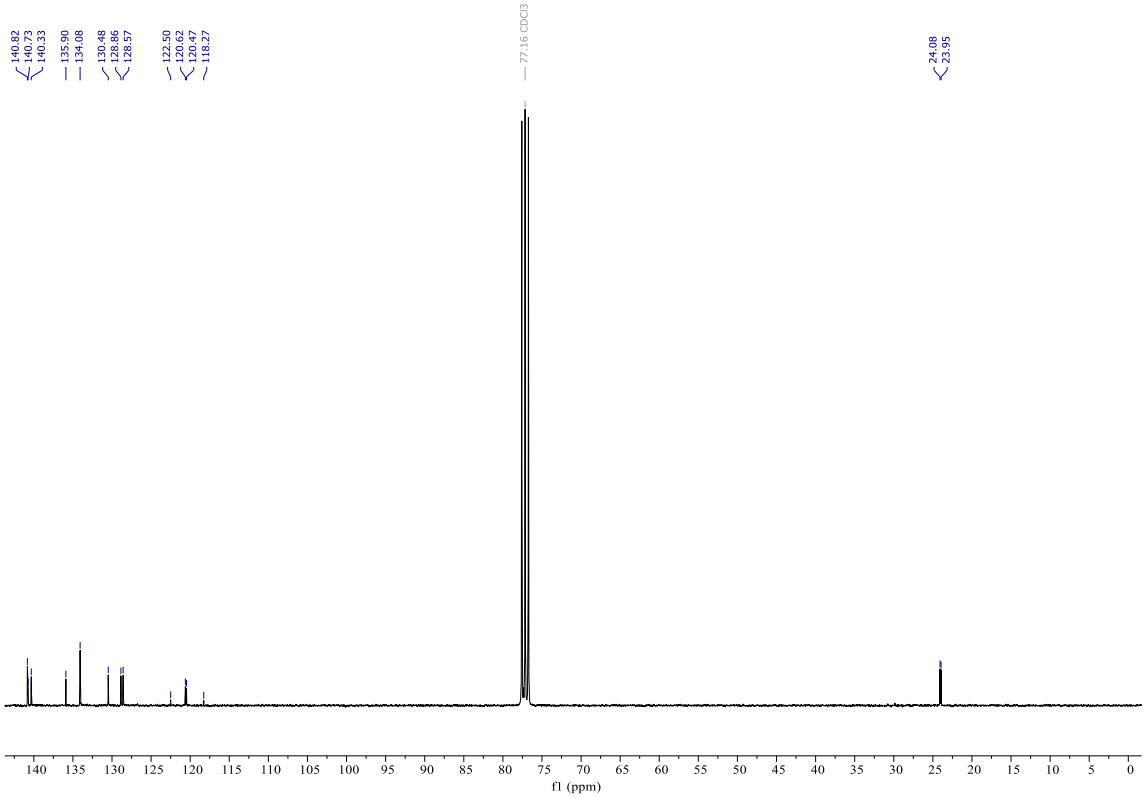
^{1}H-NMR spectrum of **25**. 600 MHz, $CDCl_3$



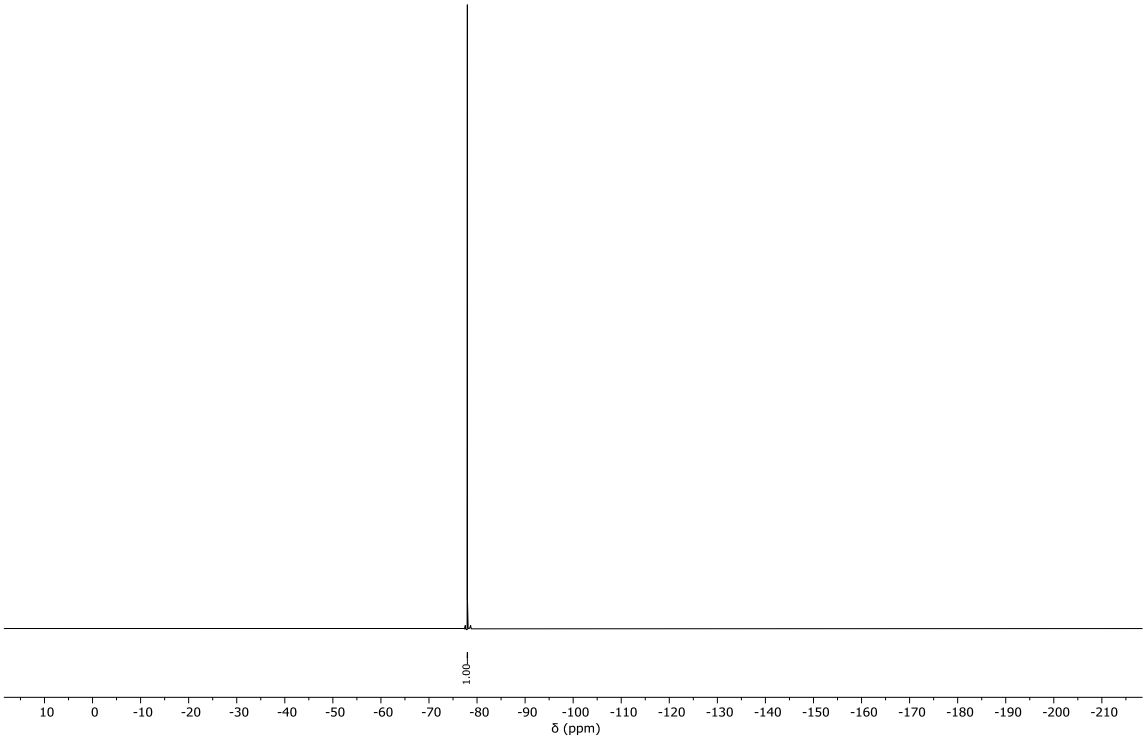
^{13}C-NMR spectrum of **25**. 151 MHz, $CDCl_3$



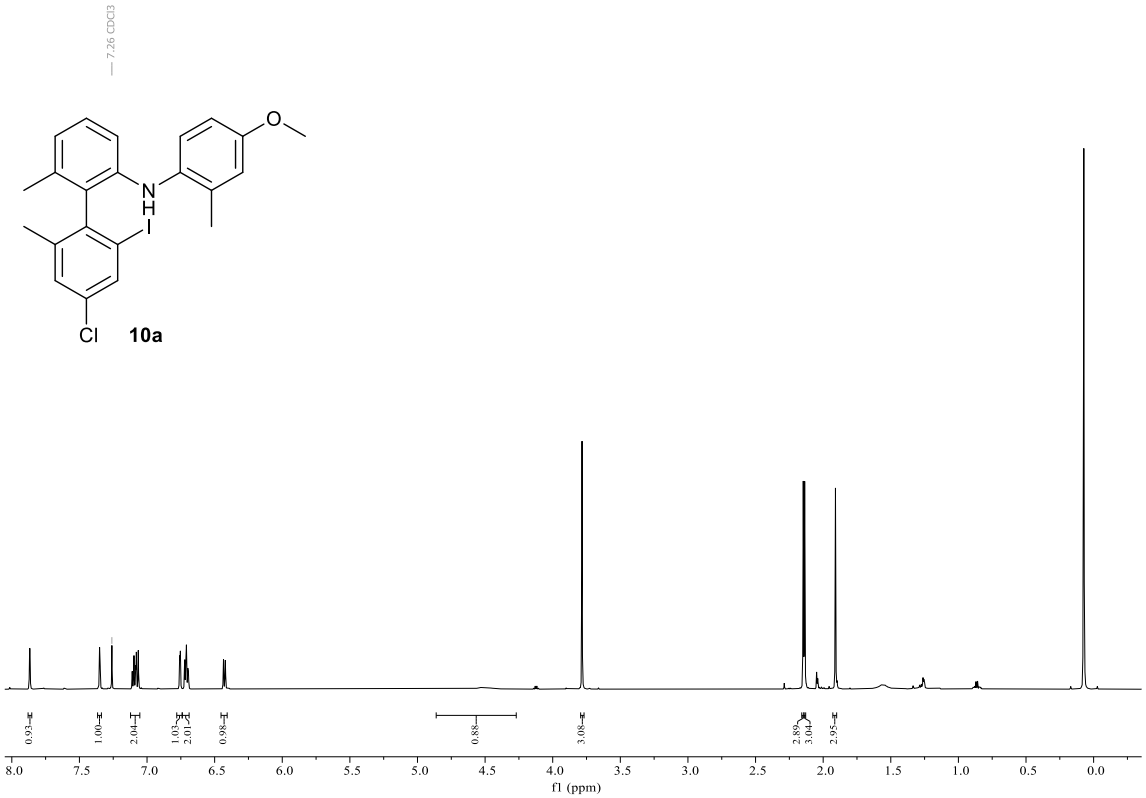
^{1}H-NMR spectrum of **9**. 600 MHz, $CDCl_3$



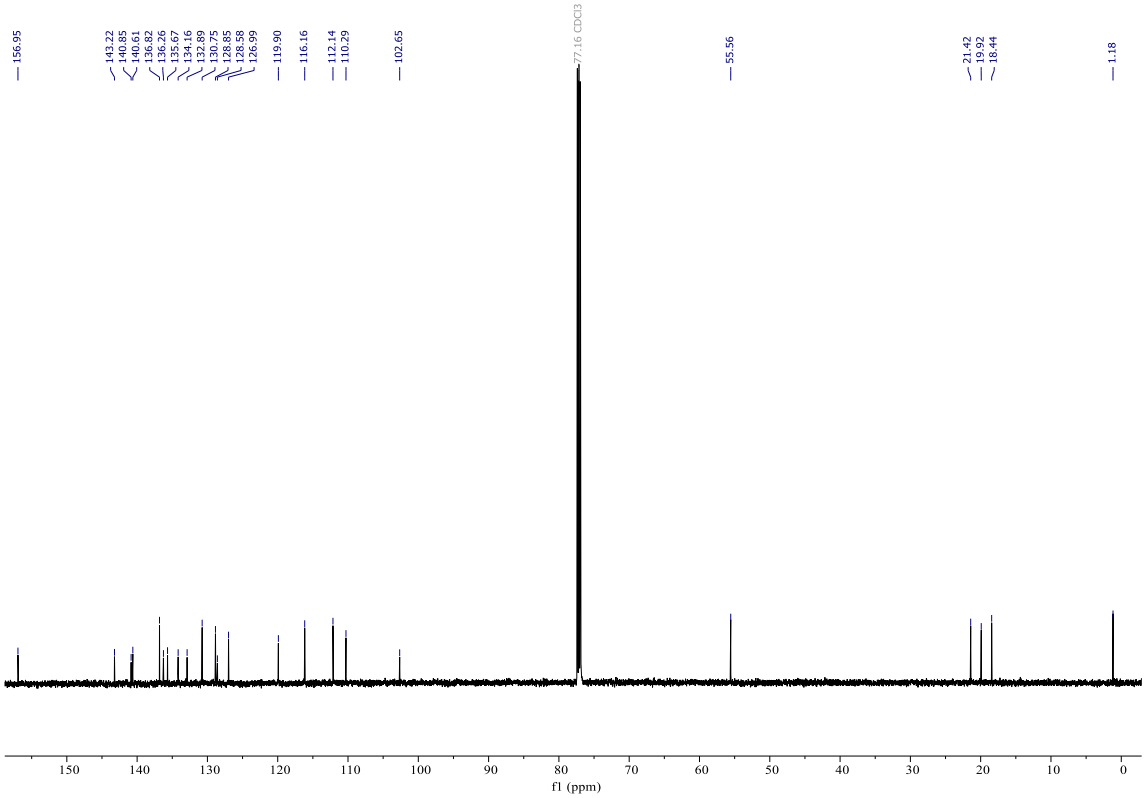
^{13}C-NMR spectrum of **9**. 75.5 MHz, $CDCl_3$



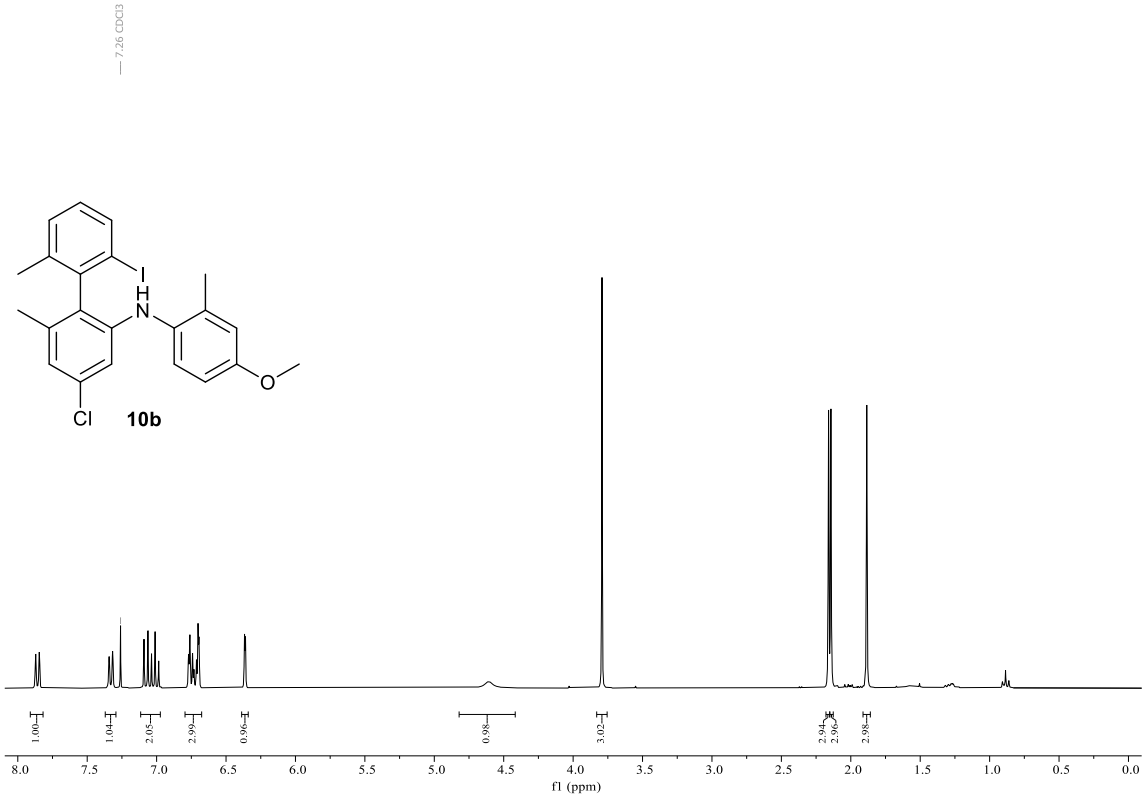
^{19}F-NMR spectrum of **9**. 282 MHz, $CDCl_3$



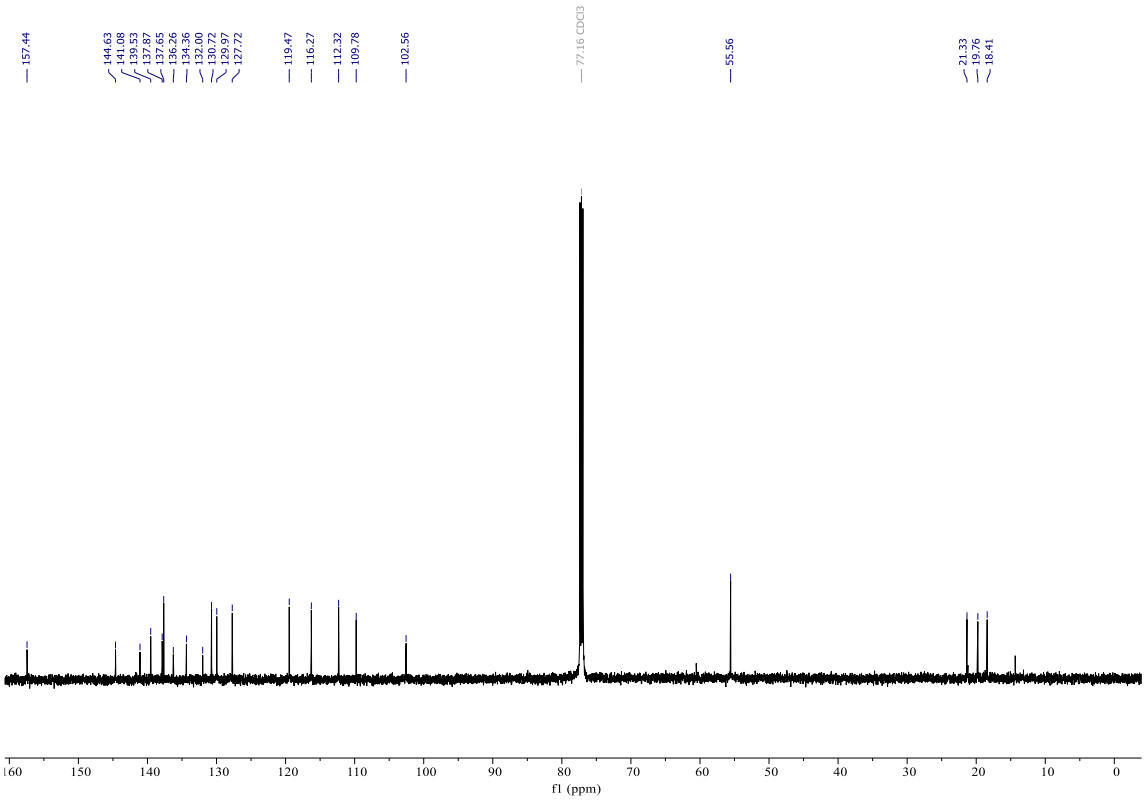
^{1}H-NMR spectrum of **10a**. 600 MHz, $CDCl_3$



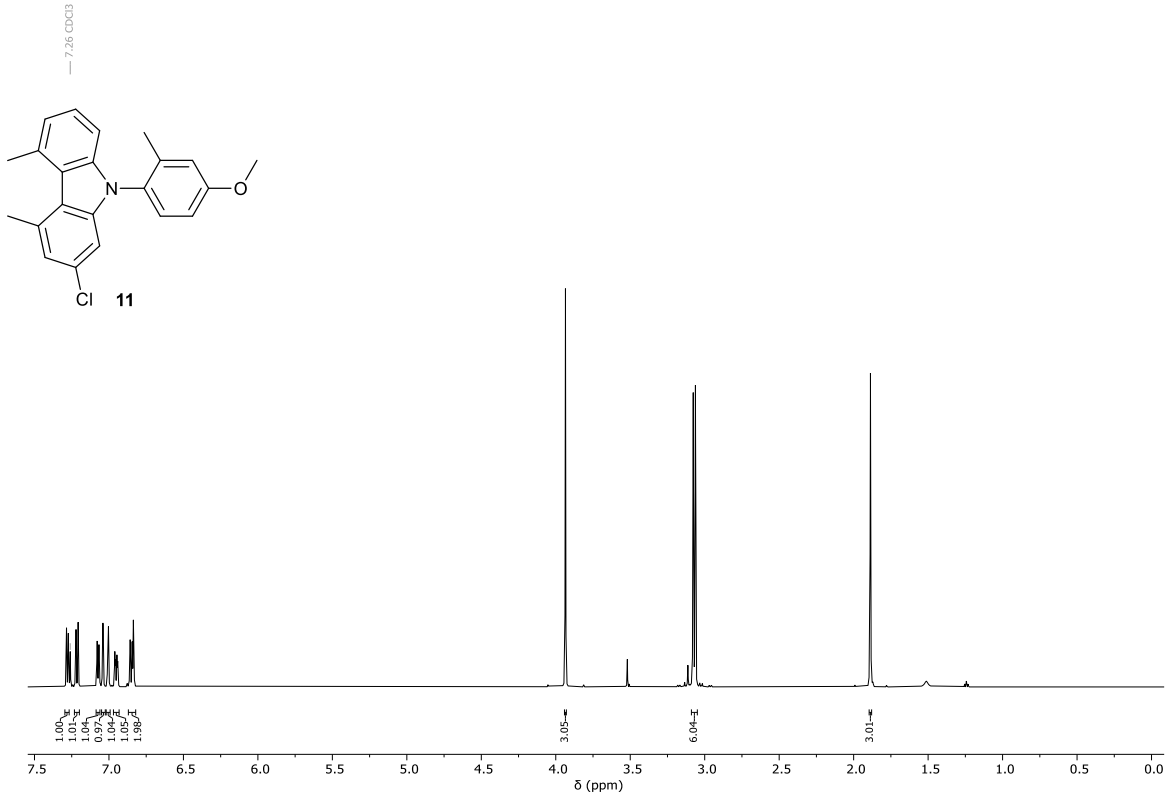
^{13}C-NMR spectrum of **10a**. 151 MHz, $CDCl_3$



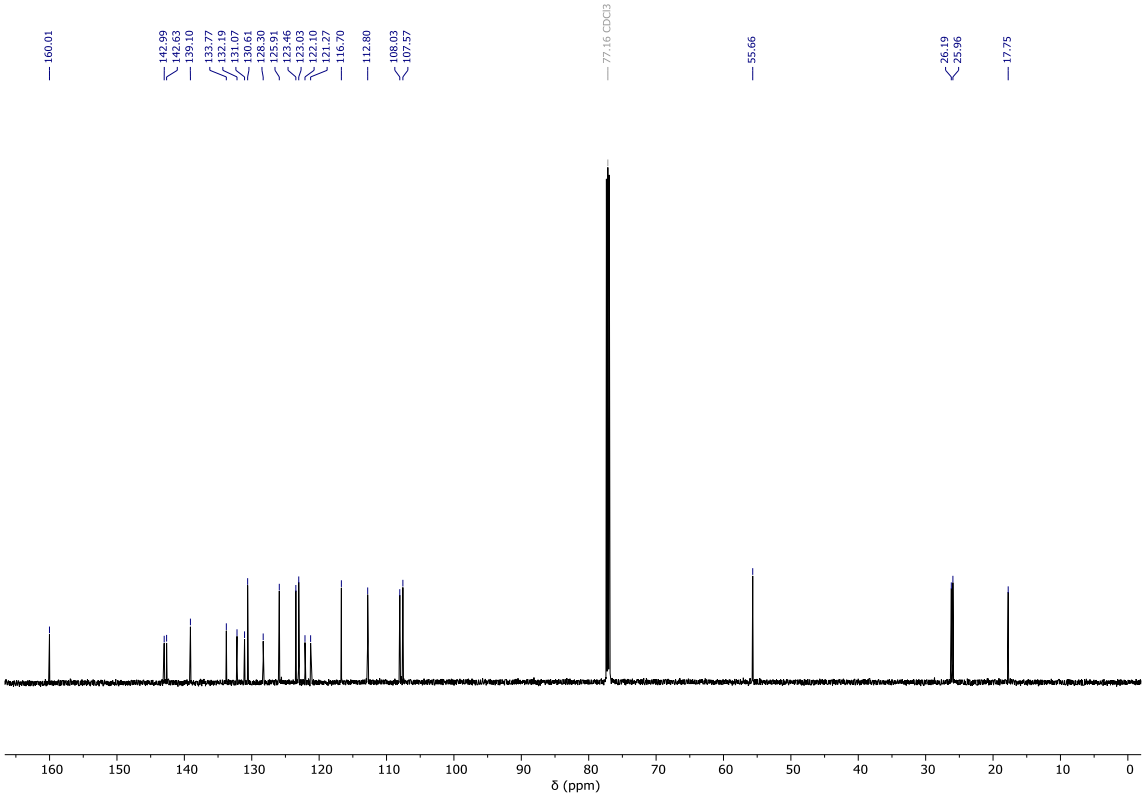
^{1}H-NMR spectrum of **10b**. 300 MHz, $CDCl_3$



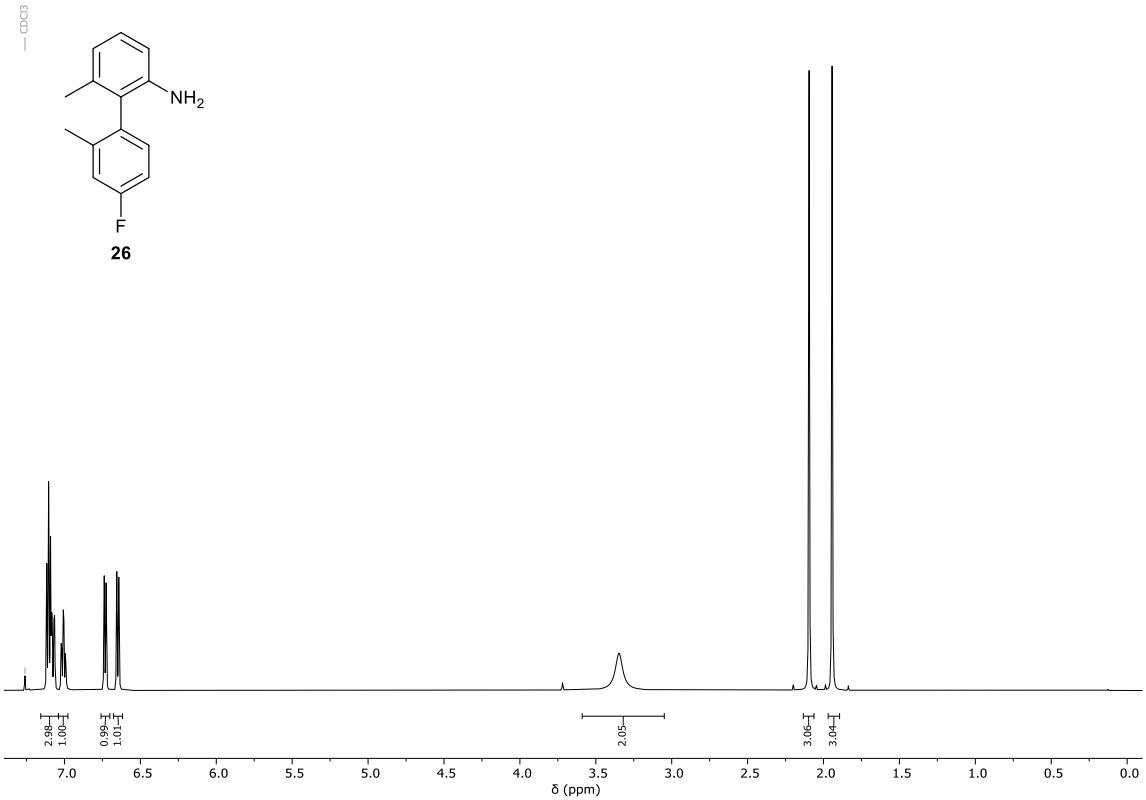
^{13}C-NMR spectrum of **10b**. 151 MHz, $CDCl_3$



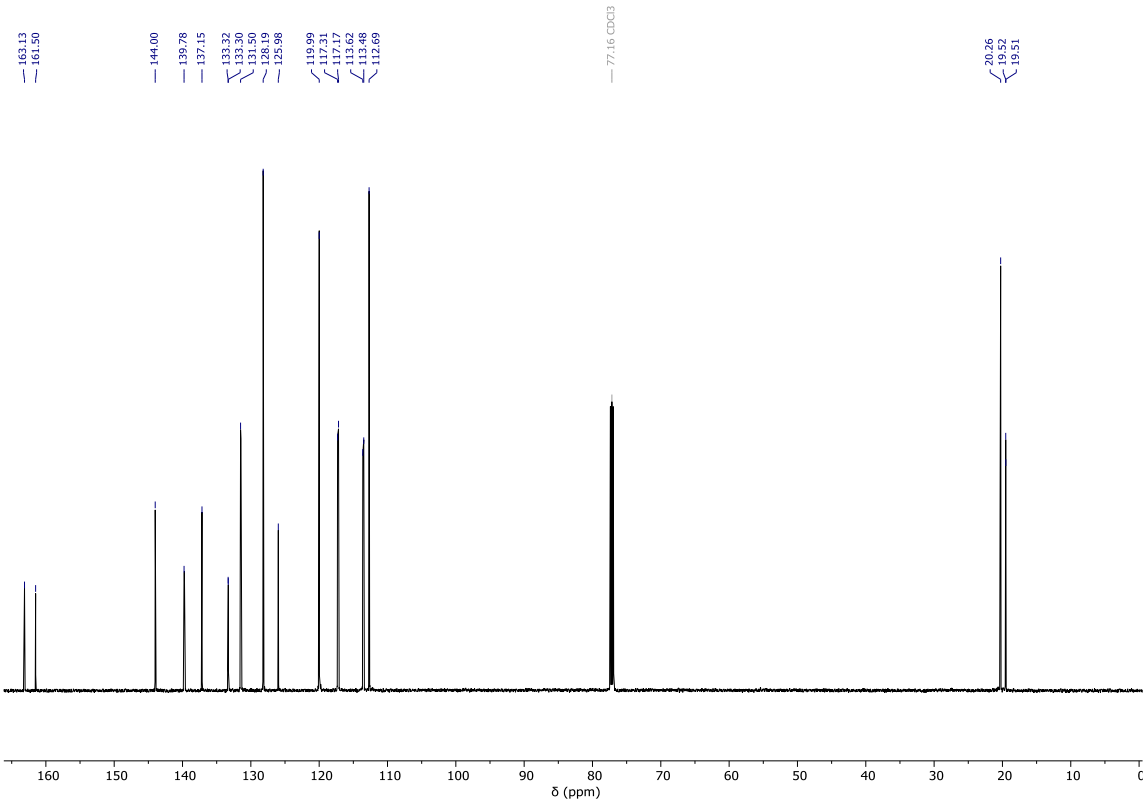
^{1}H-NMR spectrum of **11**. 600 MHz, $CDCl_3$



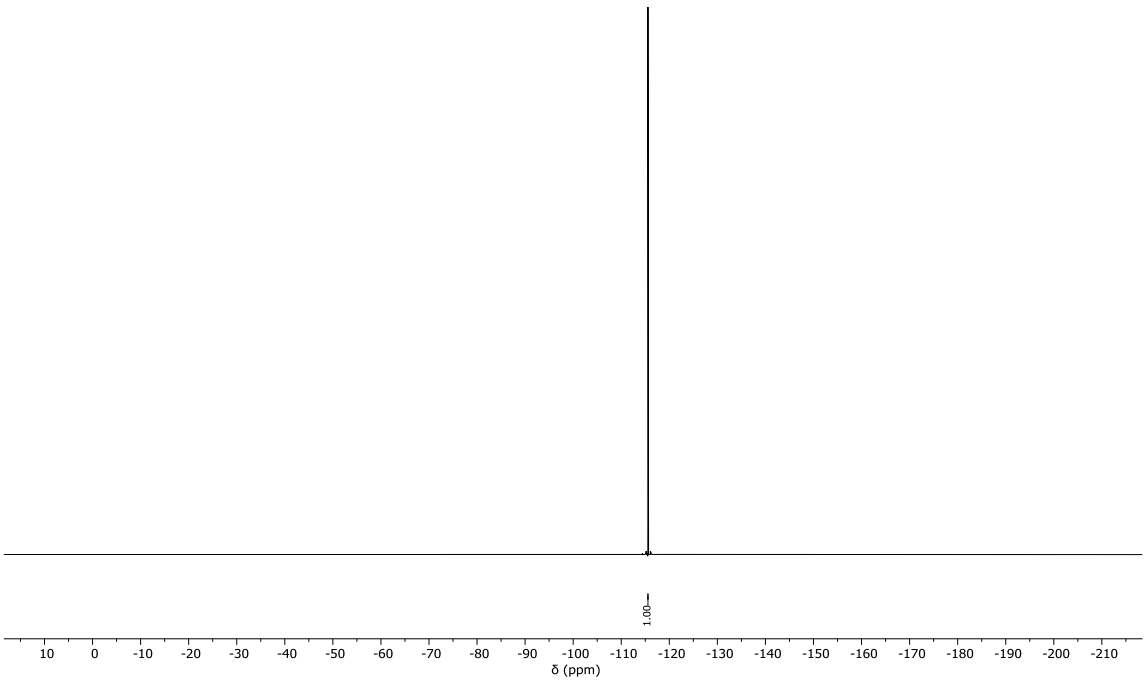
^{13}C-NMR spectrum of **11**. 151 MHz, $CDCl_3$



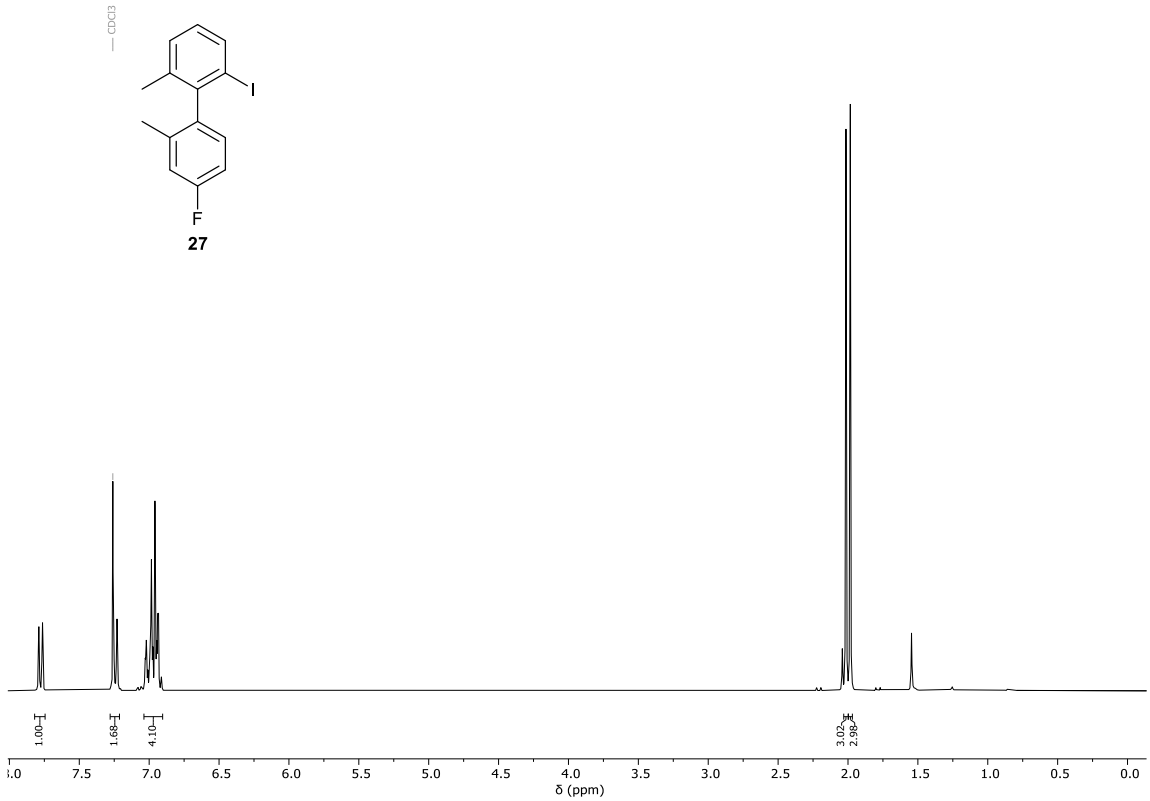
^{1}H-NMR spectrum of **26**. 600 MHz, $CDCl_3$



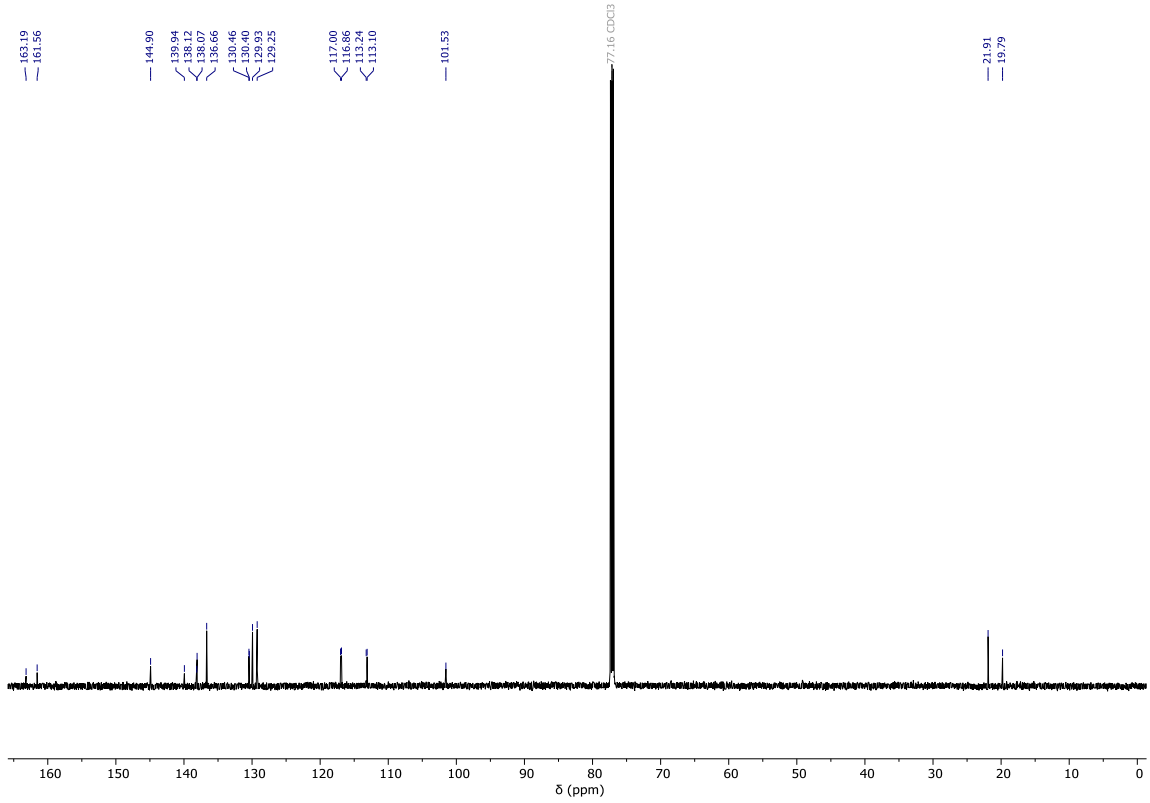
^{13}C-NMR spectrum of **26**. 151 MHz, $CDCl_3$



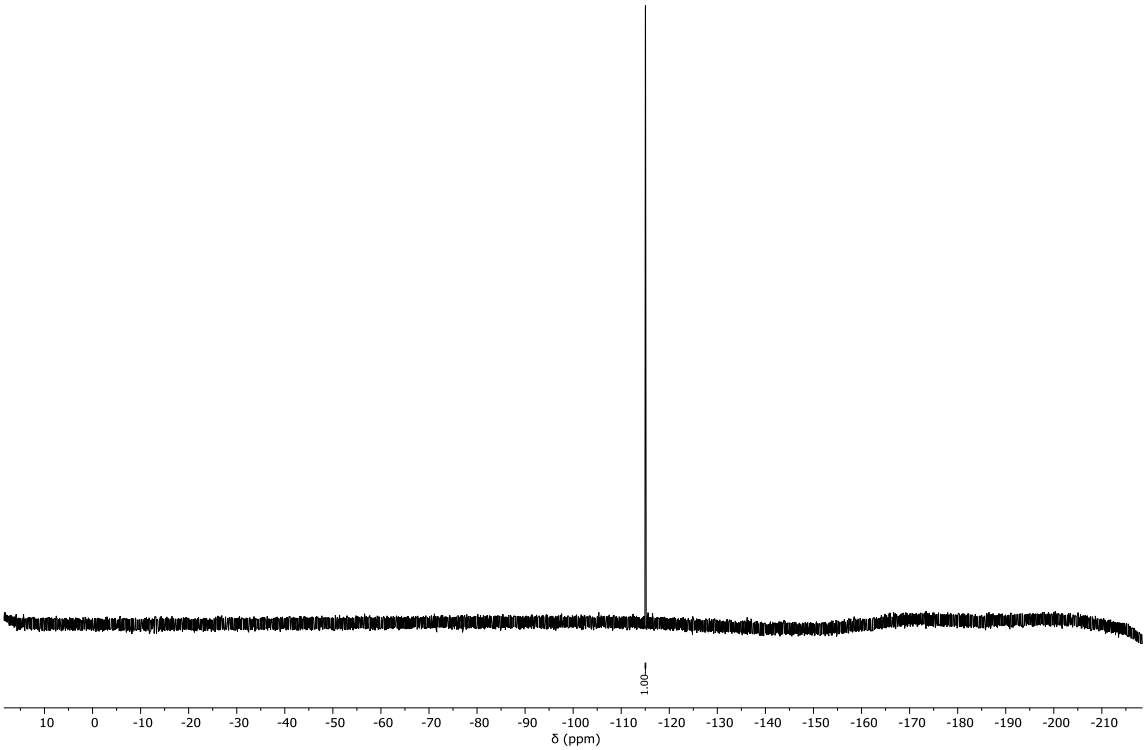
^{19}F-NMR spectrum of **26**. 282 MHz, $CDCl_3$



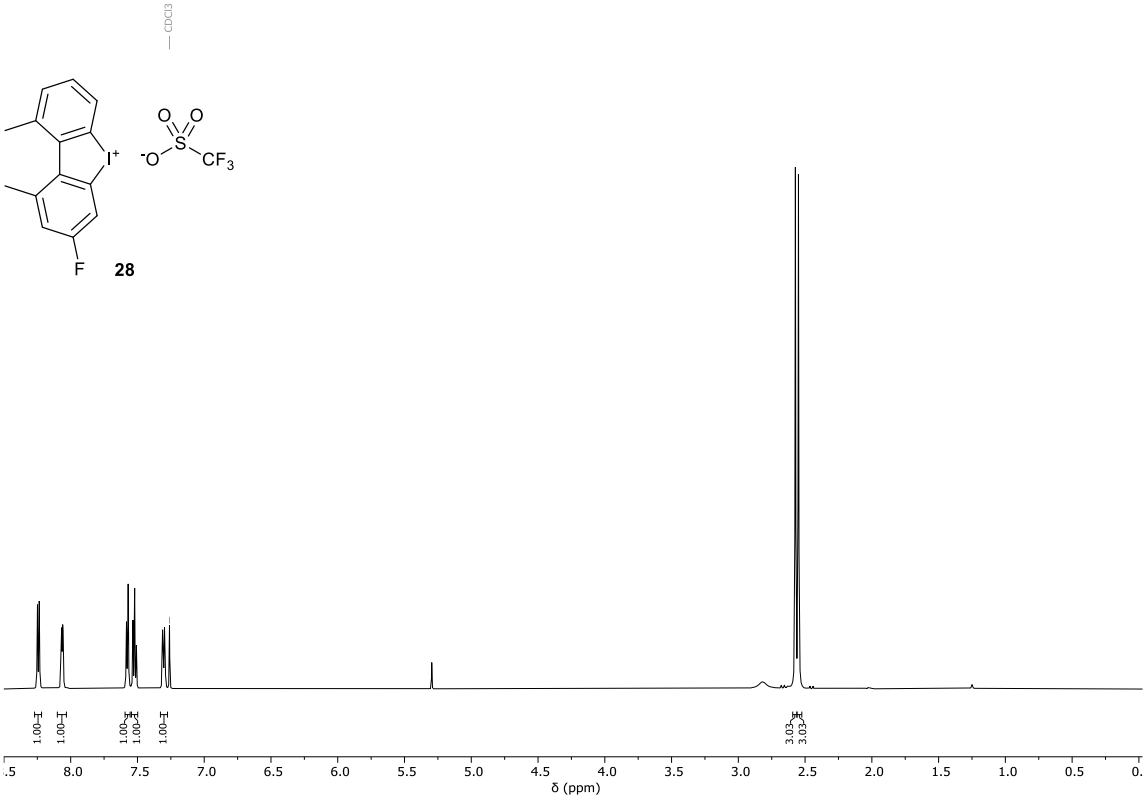
^{1}H-NMR spectrum of **27**. 600 MHz, $CDCl_3$



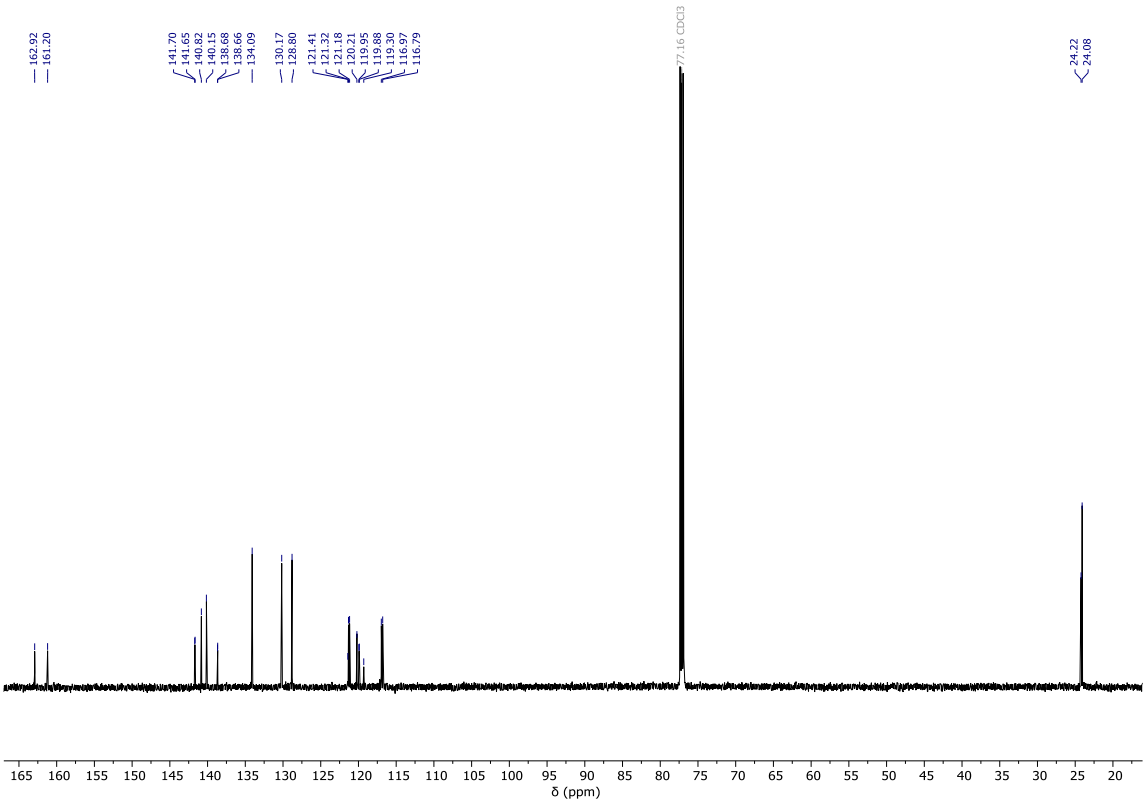
^{13}C-NMR spectrum of **27**. 151 MHz, $CDCl_3$



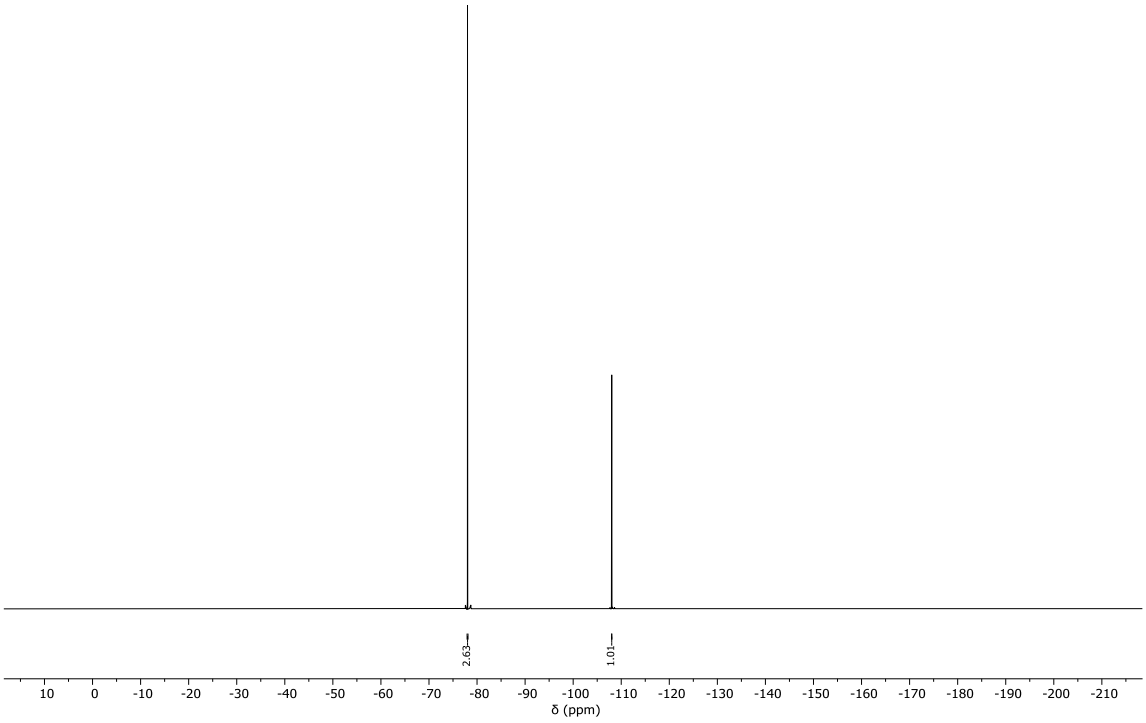
^{19}F-NMR spectrum of **27**. 282 MHz, $CDCl_3$



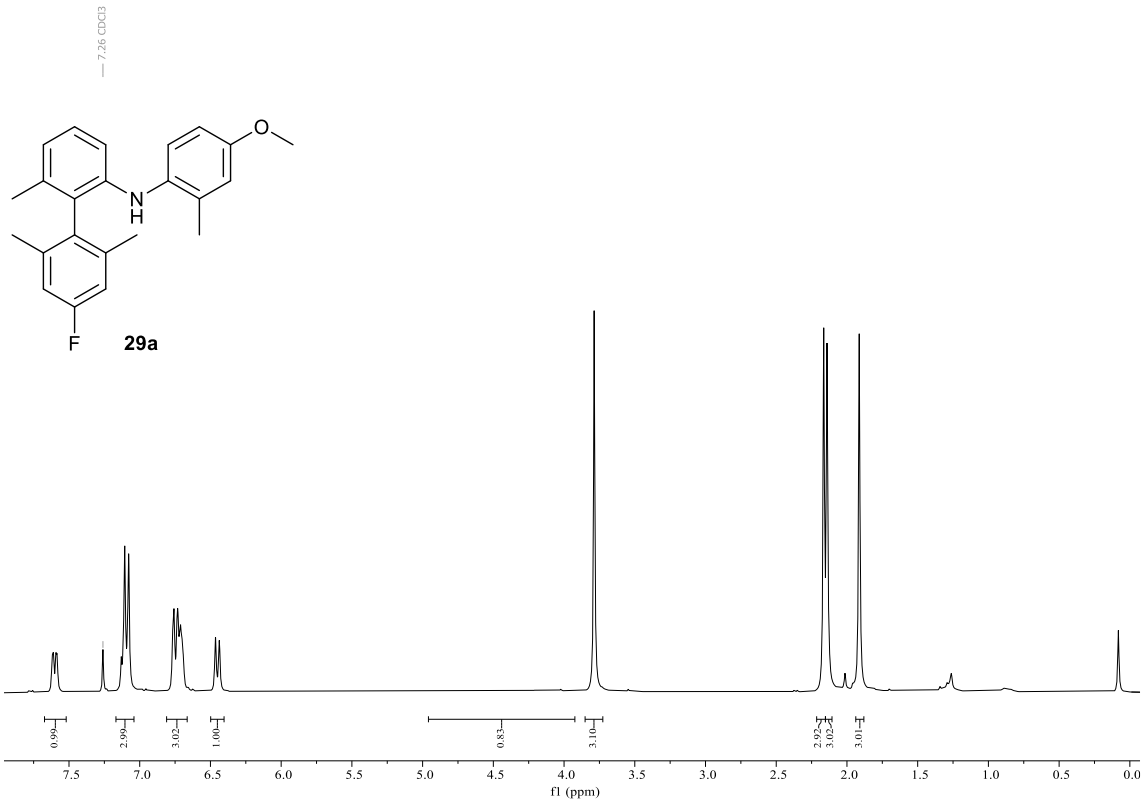
^{1}H-NMR spectrum of **28**. 600 MHz, $CDCl_3$



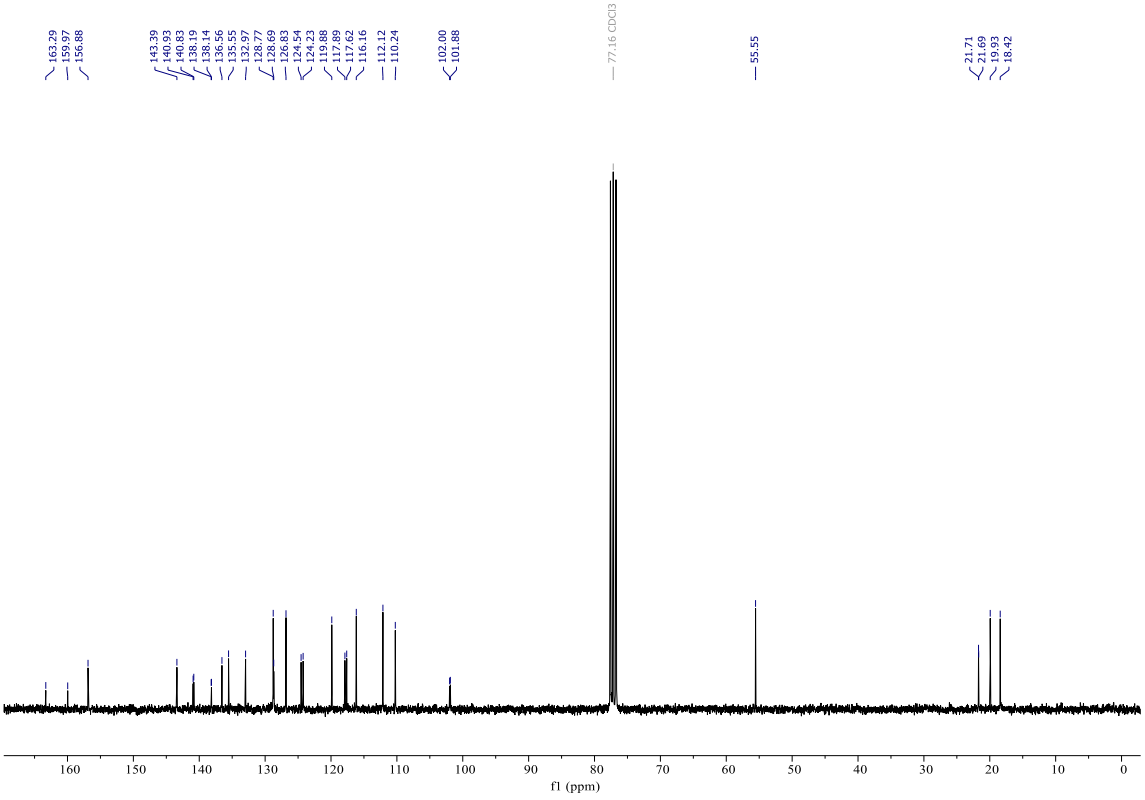
^{13}C-NMR spectrum of **28**. 151 MHz, $CDCl_3$



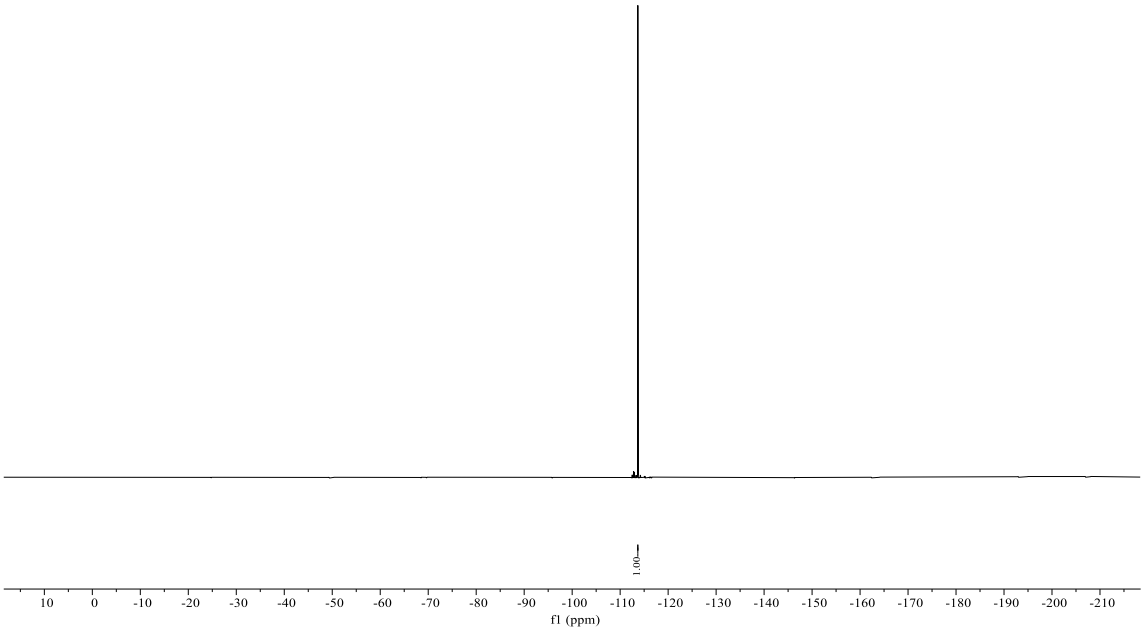
^{19}F-NMR spectrum of **28**. 282 MHz, $CDCl_3$



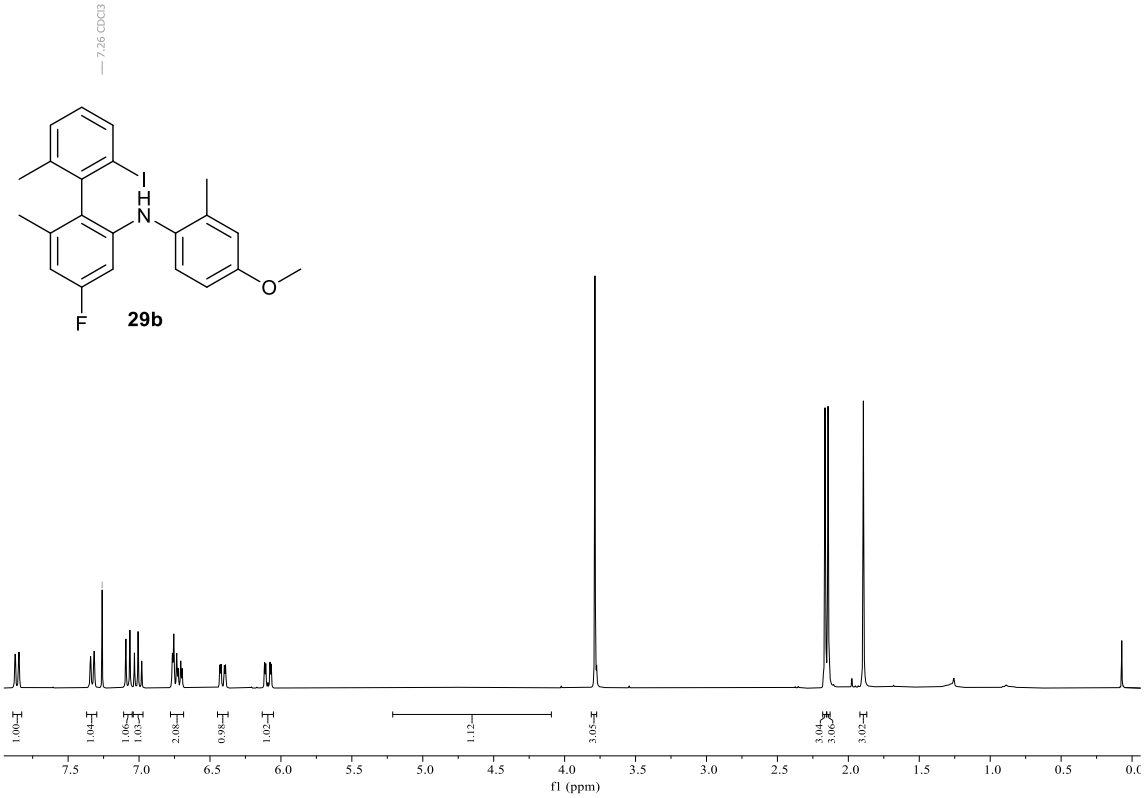
^{1}H-NMR spectrum of **29a**. 300 MHz, $CDCl_3$



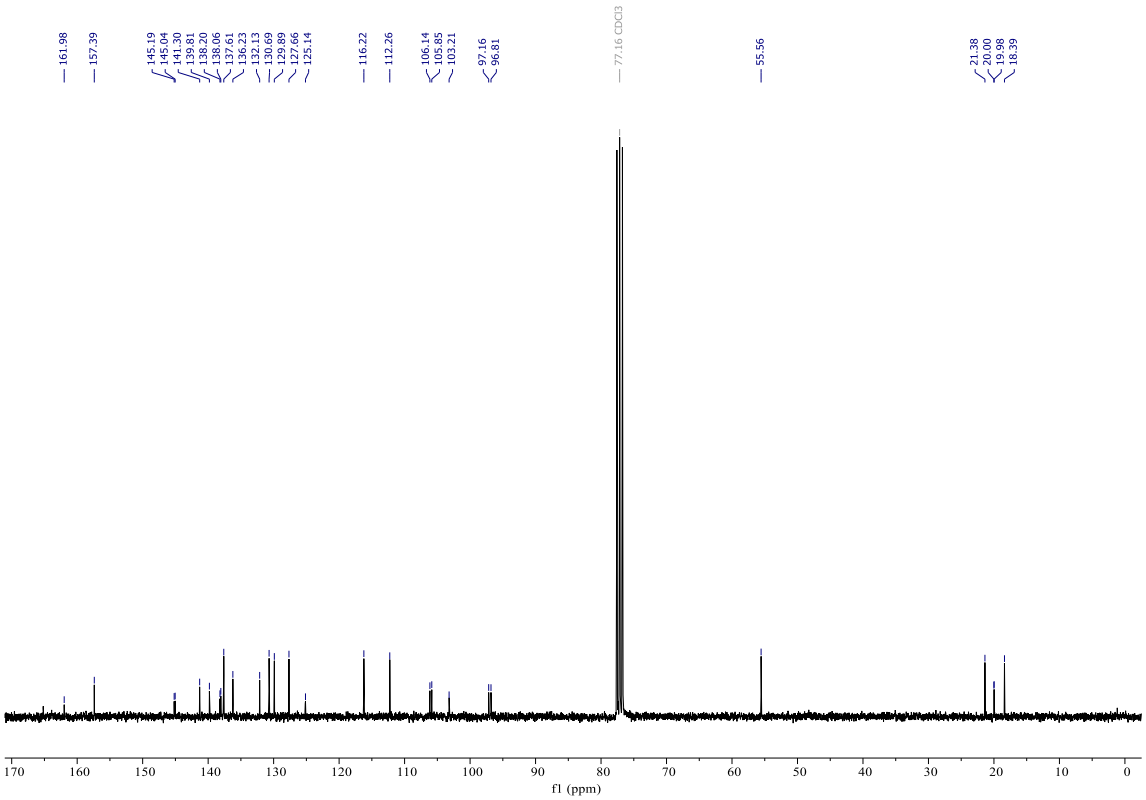
^{13}C-NMR spectrum of **29a**. 75.5 MHz, $CDCl_3$



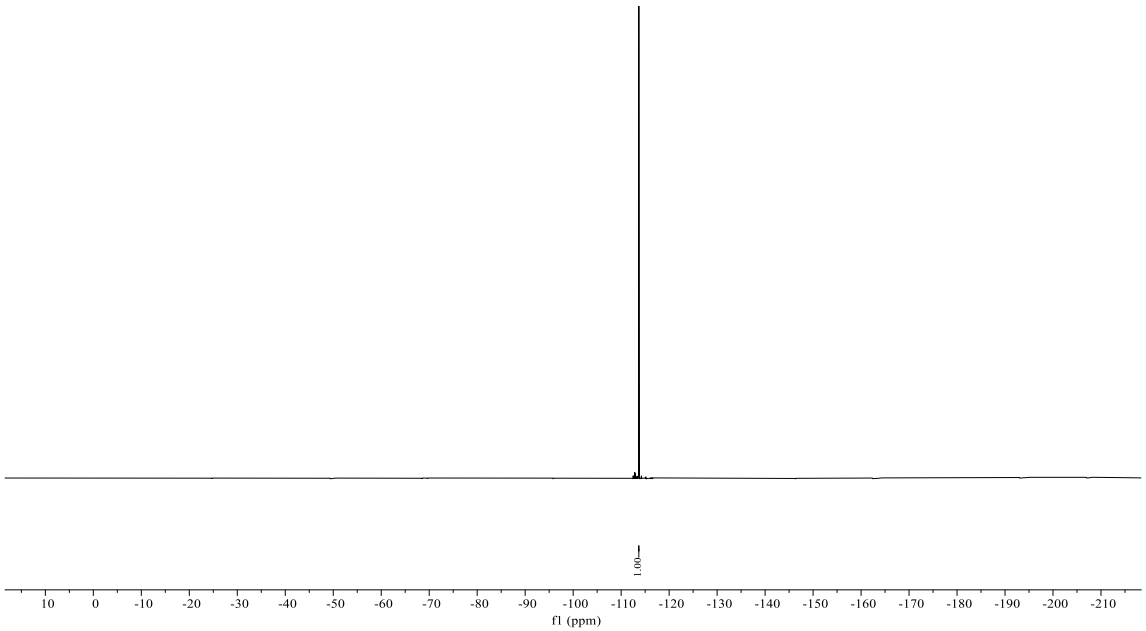
^{19}F-NMR spectrum of **29a**. 282 MHz, $CDCl_3$



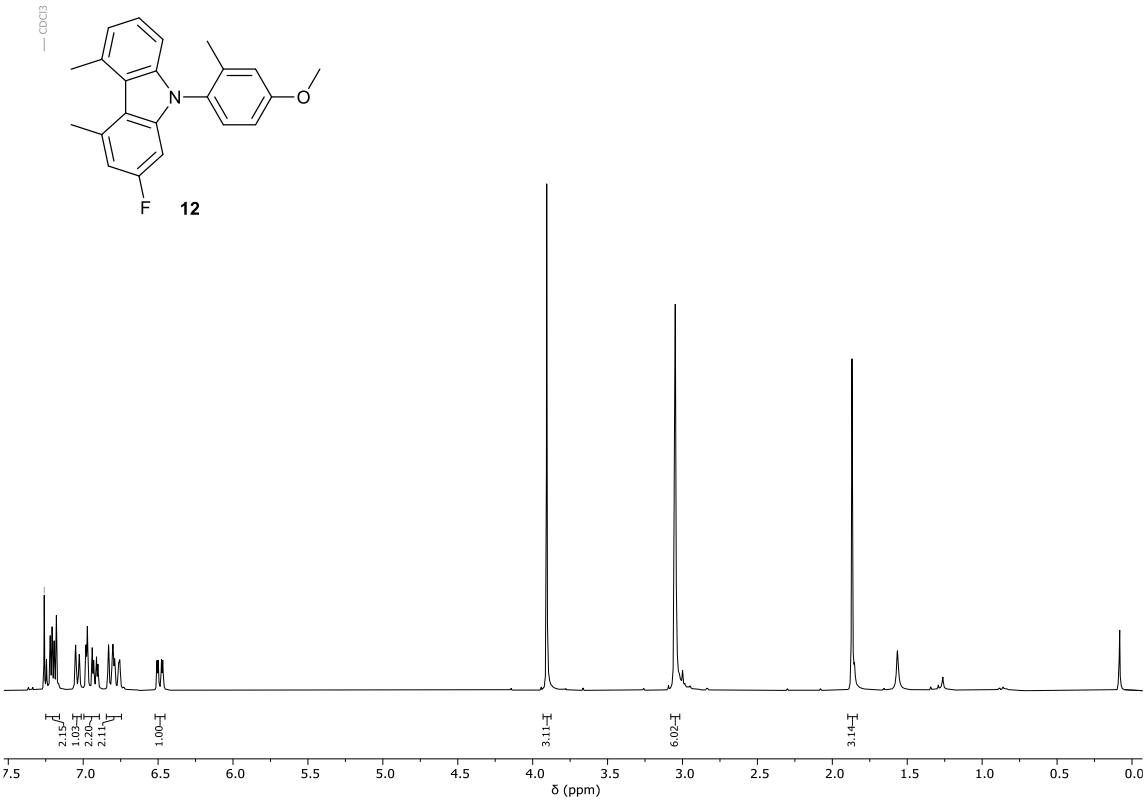
^{1}H-NMR spectrum of **29b**. 300 MHz, $CDCl_3$



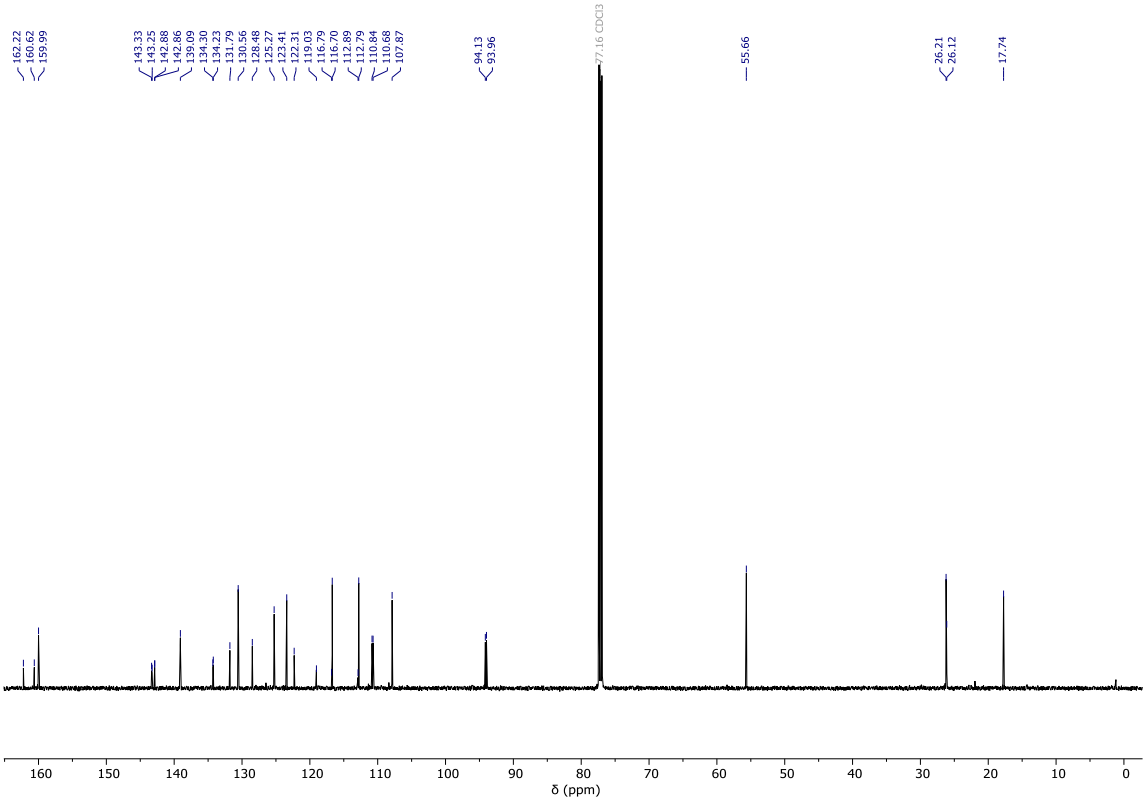
^{13}C-NMR spectrum of **29b**. 75.5 MHz, $CDCl_3$



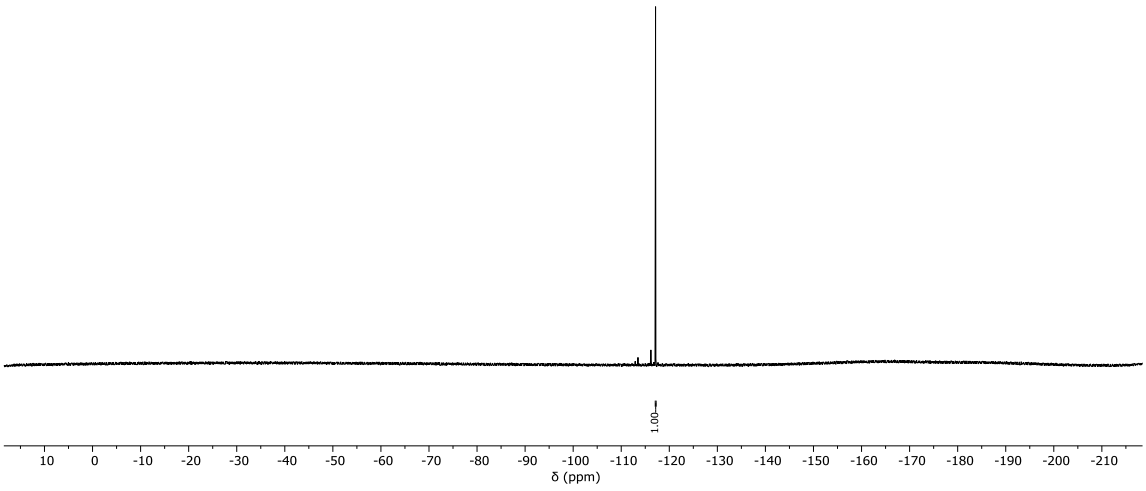
^{19}F-NMR spectrum of **29b**. 282 MHz, $CDCl_3$



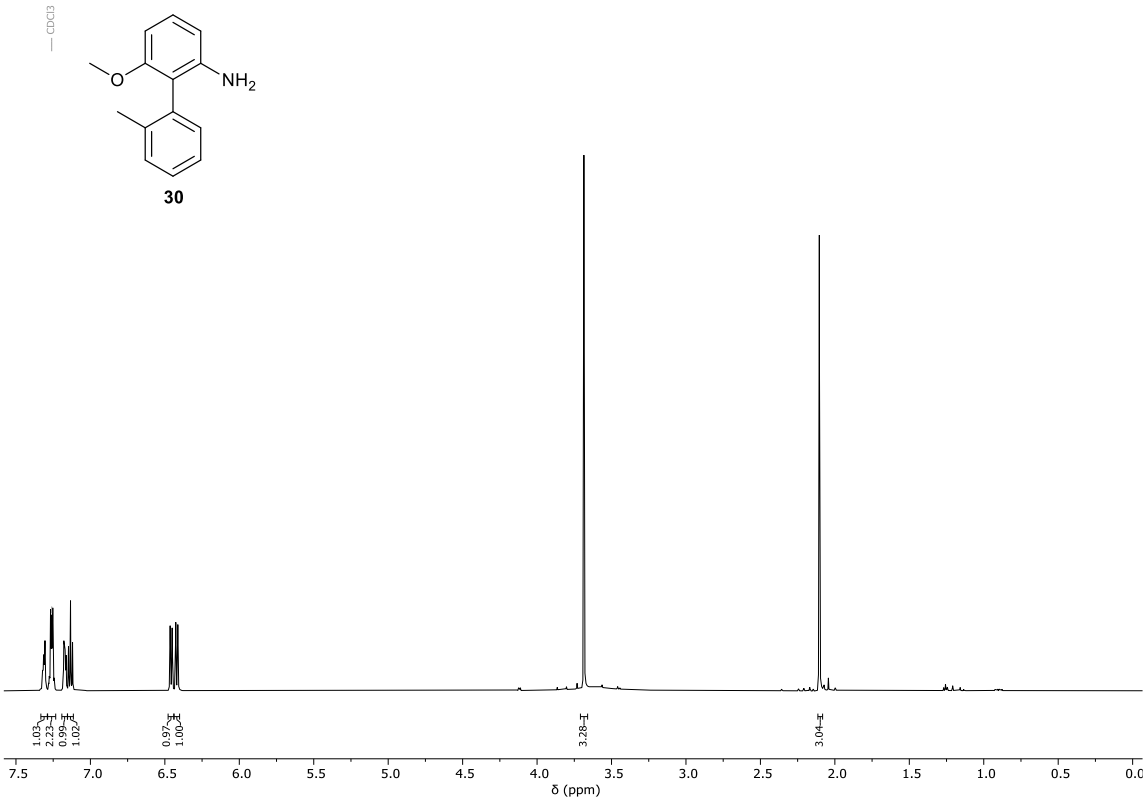
^{1}H-NMR spectrum of **12**. 600 MHz, $CDCl_3$



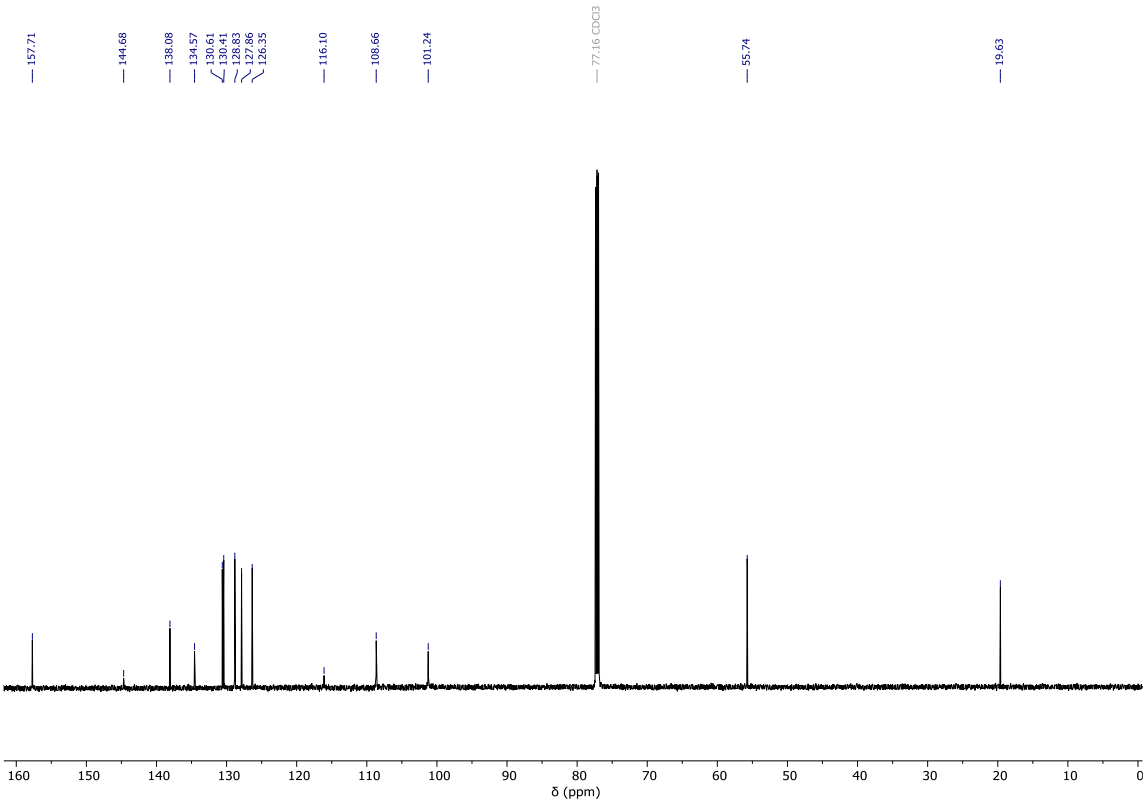
^{13}C-NMR spectrum of **12**. 151 MHz, $CDCl_3$



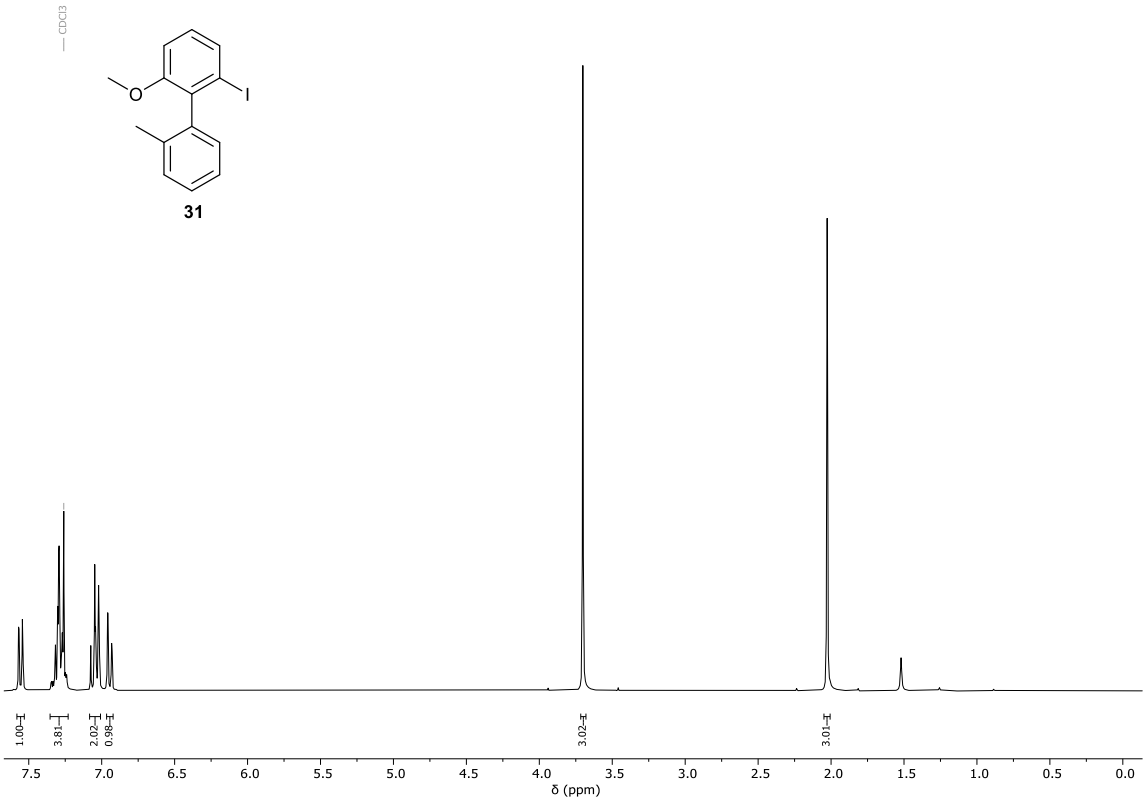
^{19}F-NMR spectrum of **12**. 282 MHz, $CDCl_3$



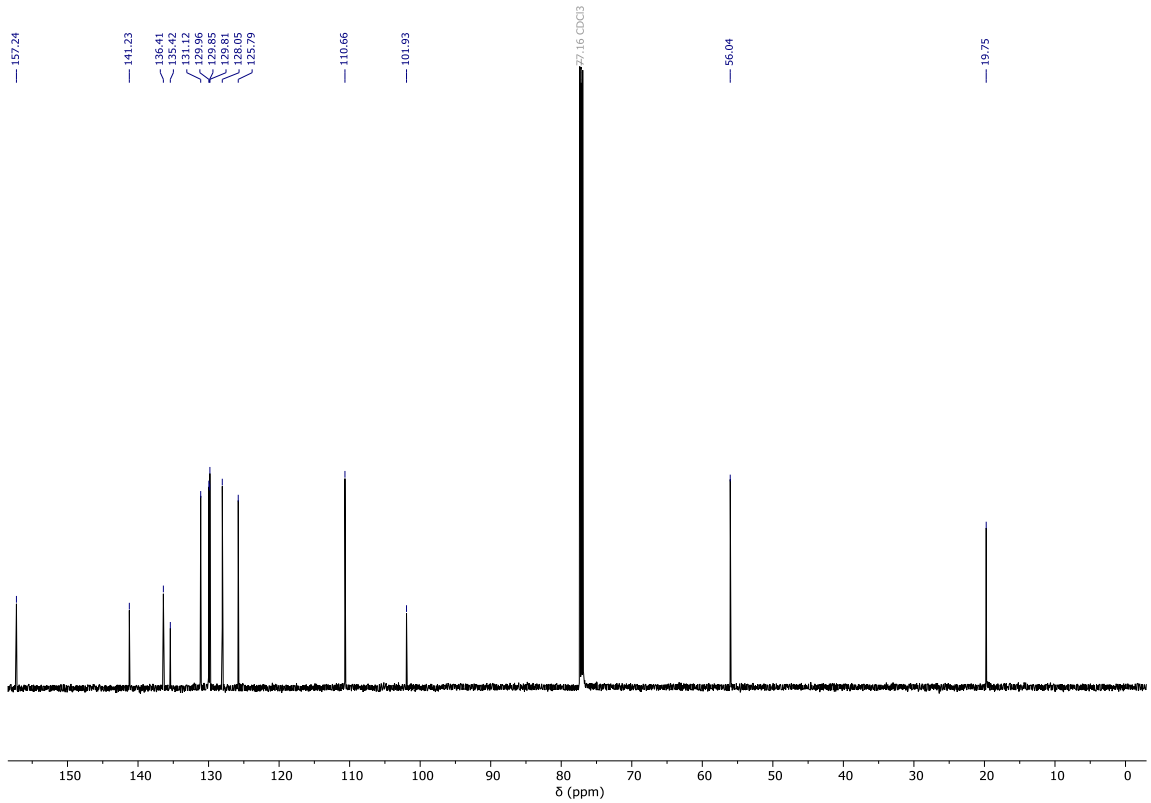
^{1}H-NMR spectrum of **30**. 600 MHz, $CDCl_3$



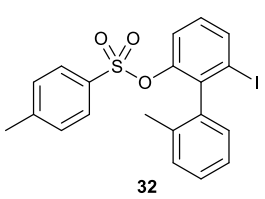
^{13}C-NMR spectrum of **30**. 151 MHz, $CDCl_3$



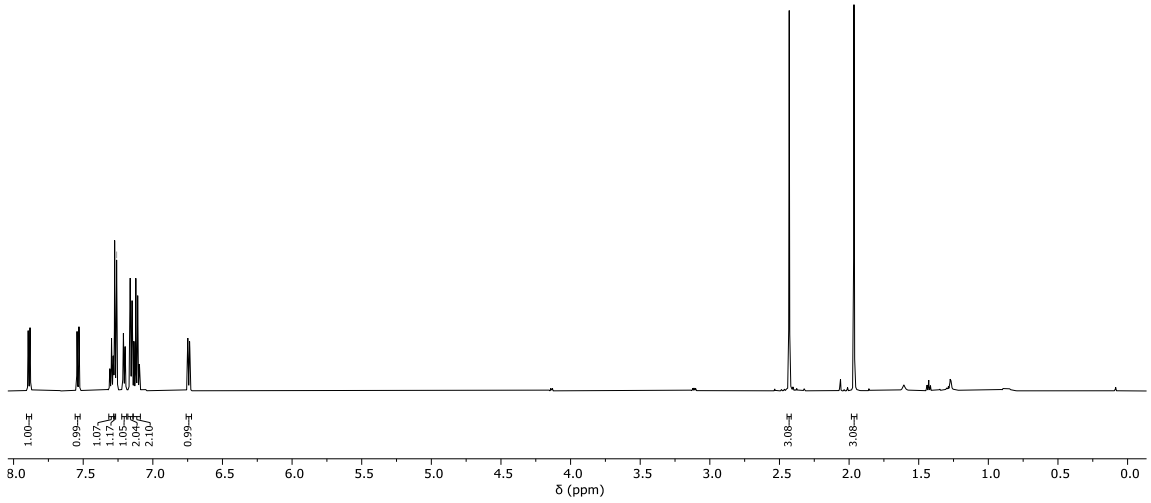
^{1}H-NMR spectrum of **31**. 300 MHz, $CDCl_3$



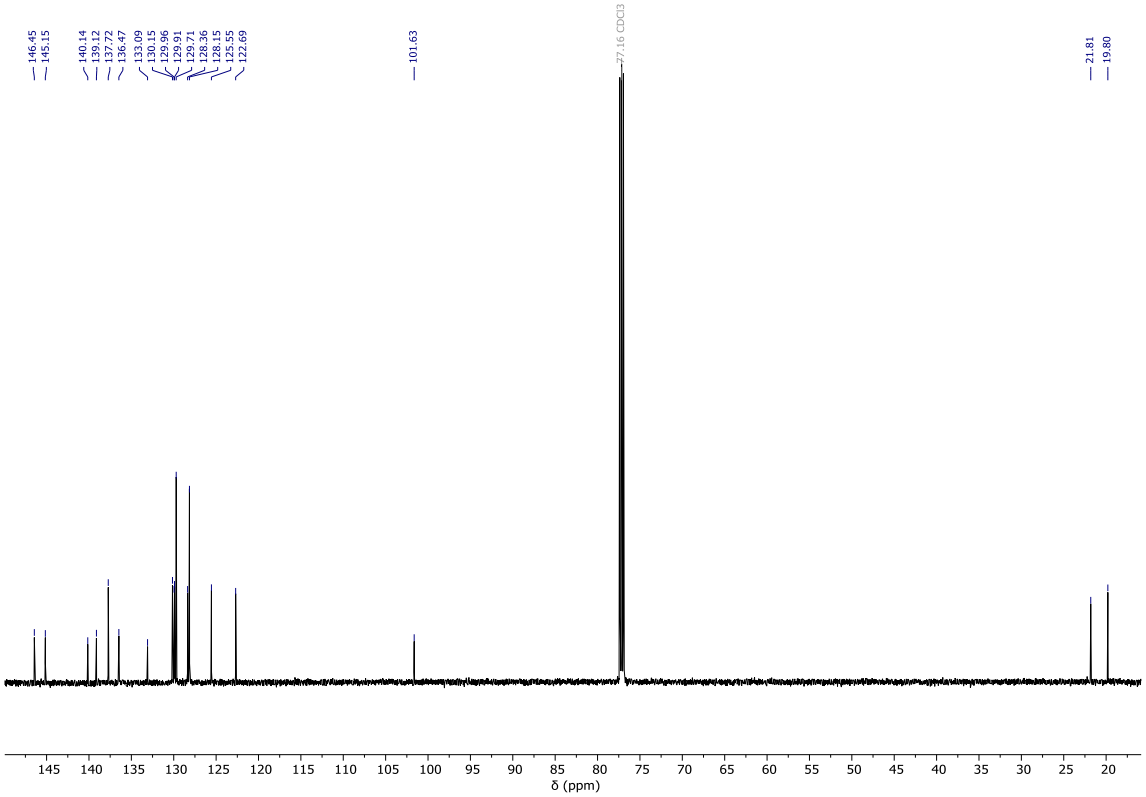
^{13}C-NMR spectrum of **31**. 151 MHz, $CDCl_3$



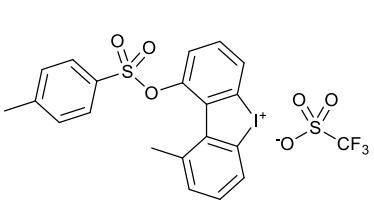
32



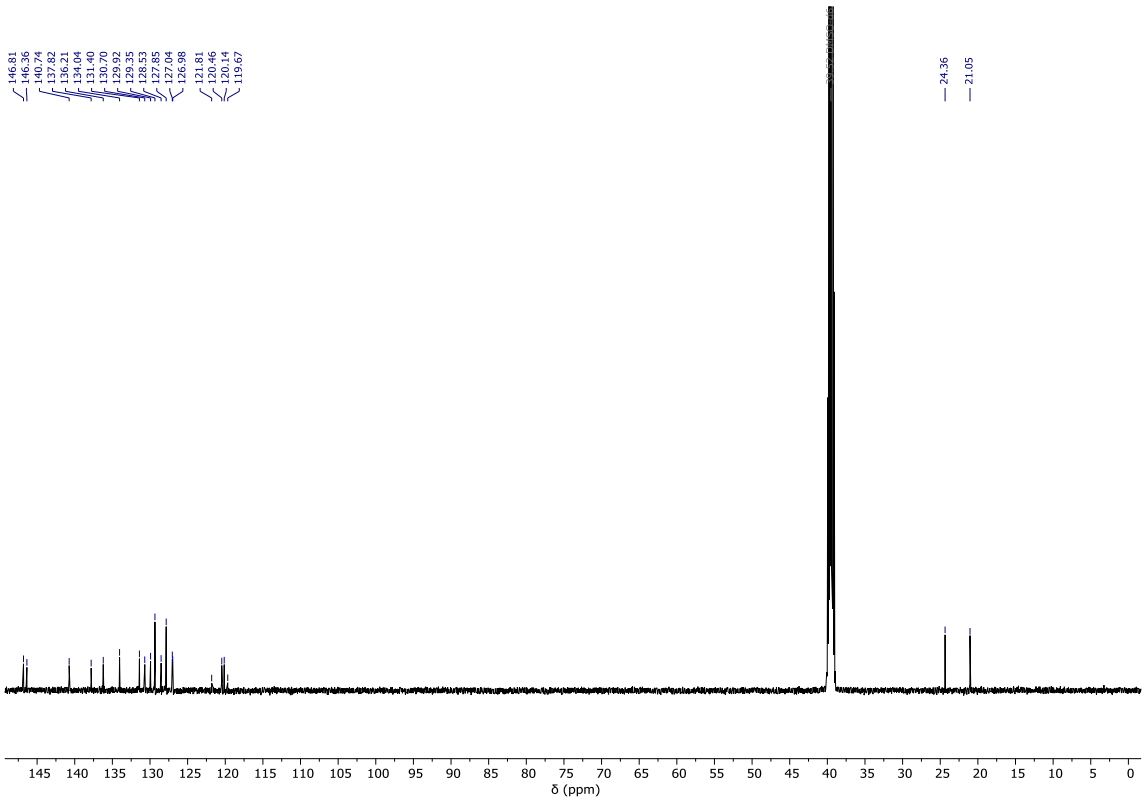
^{1}H-NMR spectrum of **32**. 600 MHz, $CDCl_3$



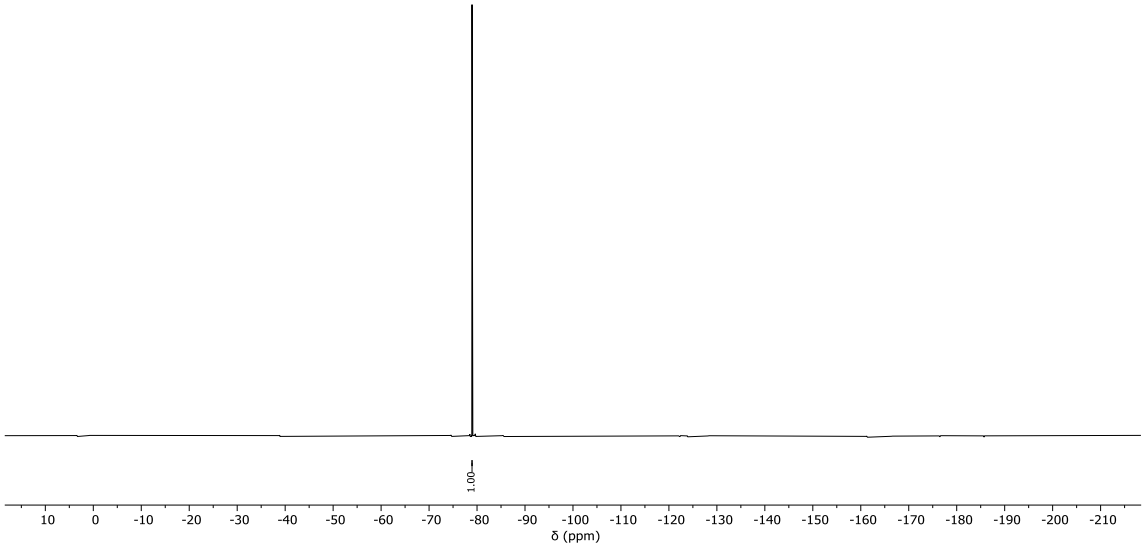
^{13}C-NMR spectrum of **32**. 151 MHz, $CDCl_3$



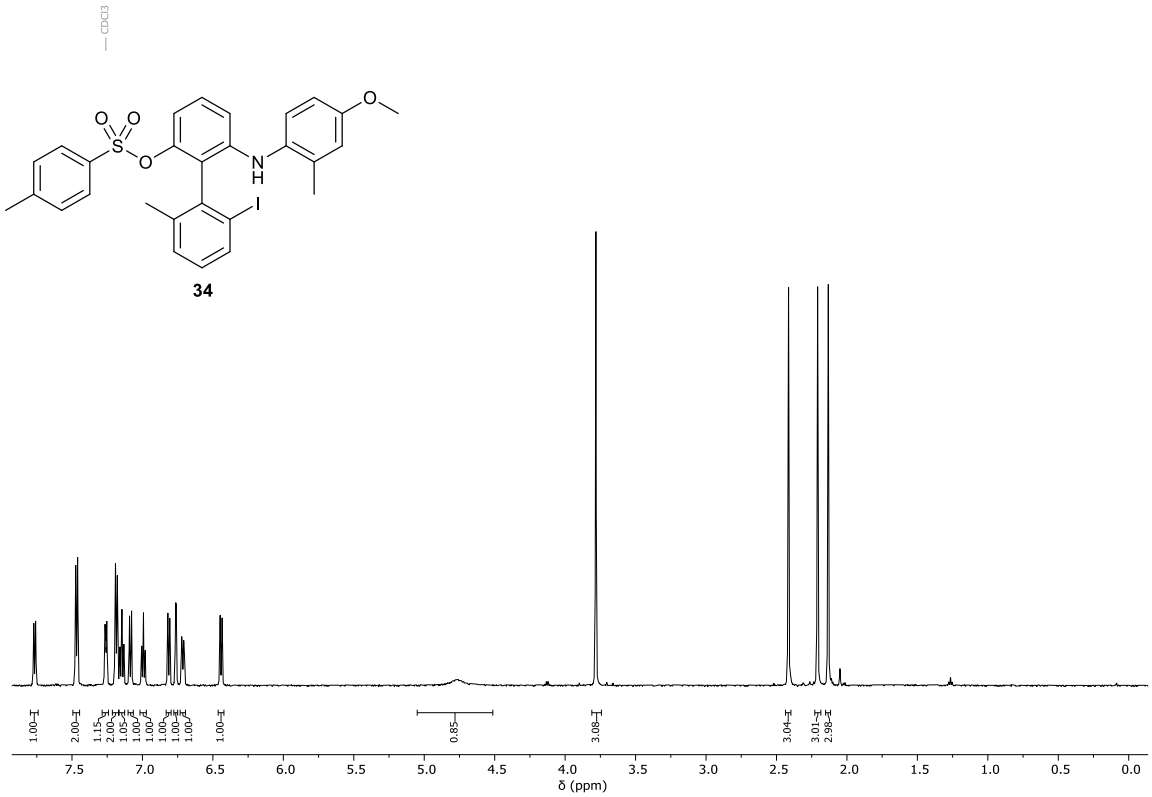
^{1}H-NMR spectrum of **33**. 600 MHz, $(CD_3)_2CO$



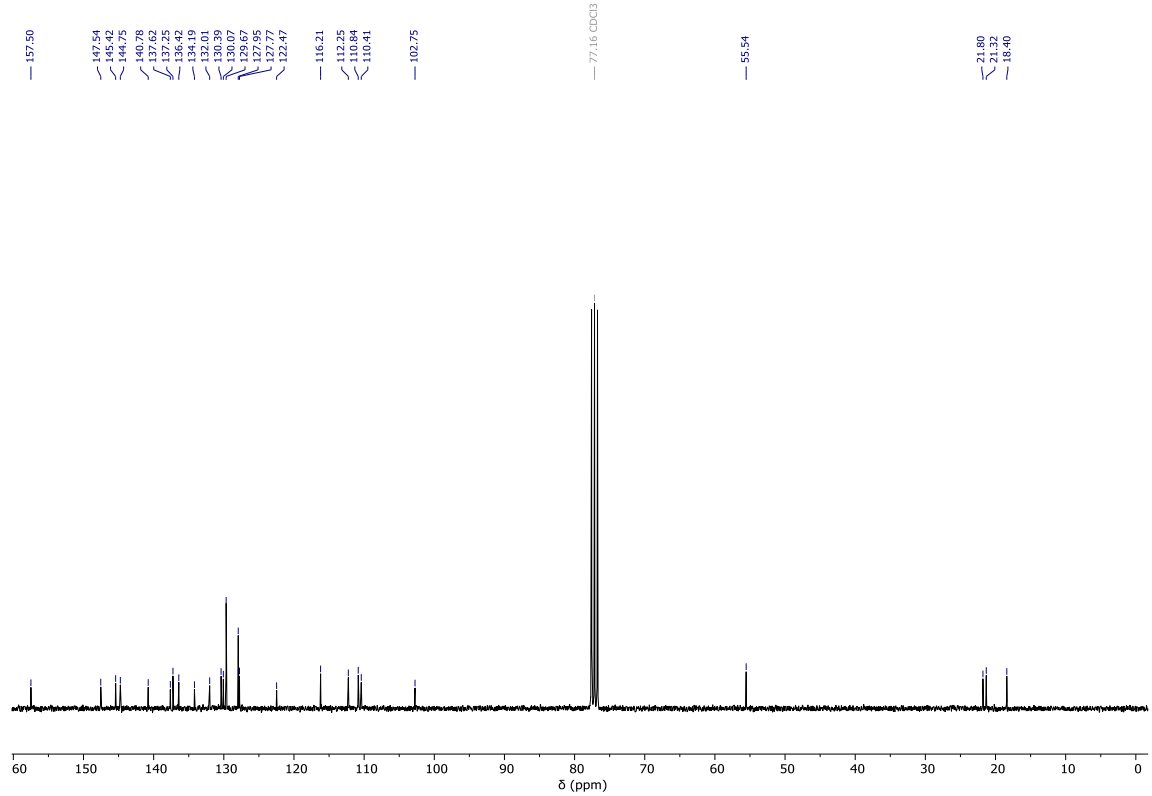
^{13}C-NMR spectrum of **33**. 151 MHz, $(CD_3)_2SO$



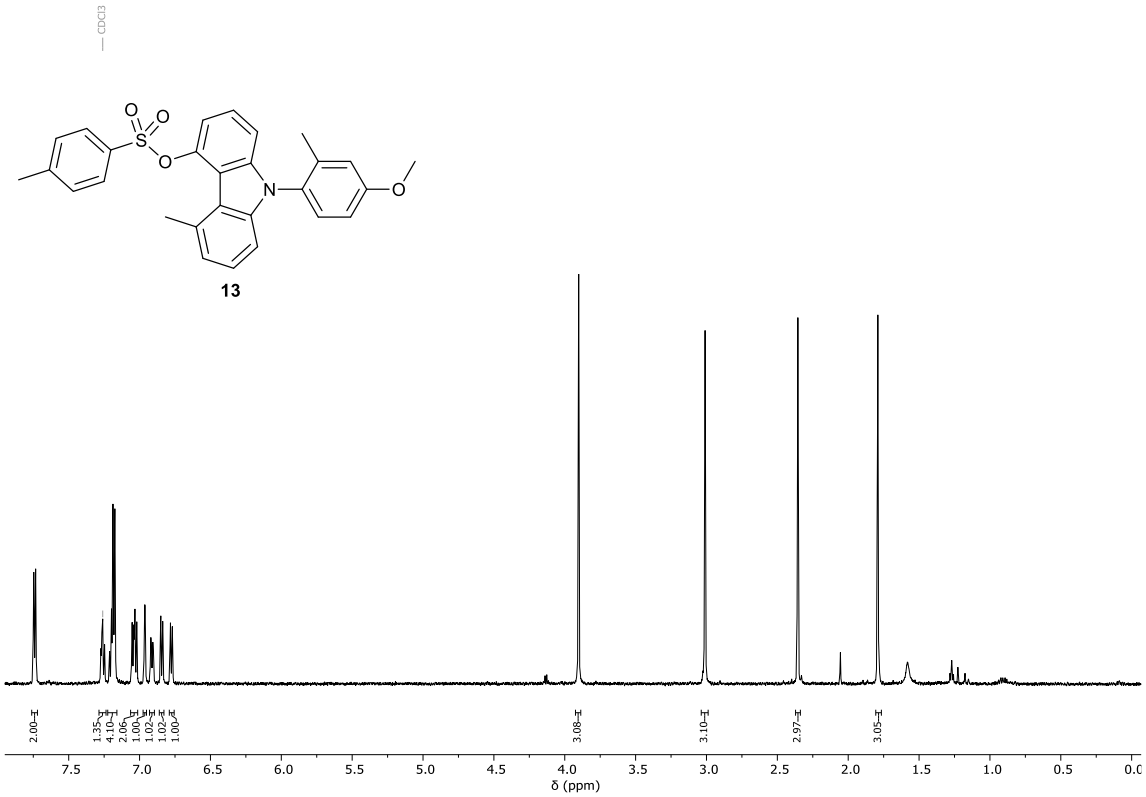
^{19}F-NMR spectrum of **33**. 282 MHz, $(CD_3)_2CO$



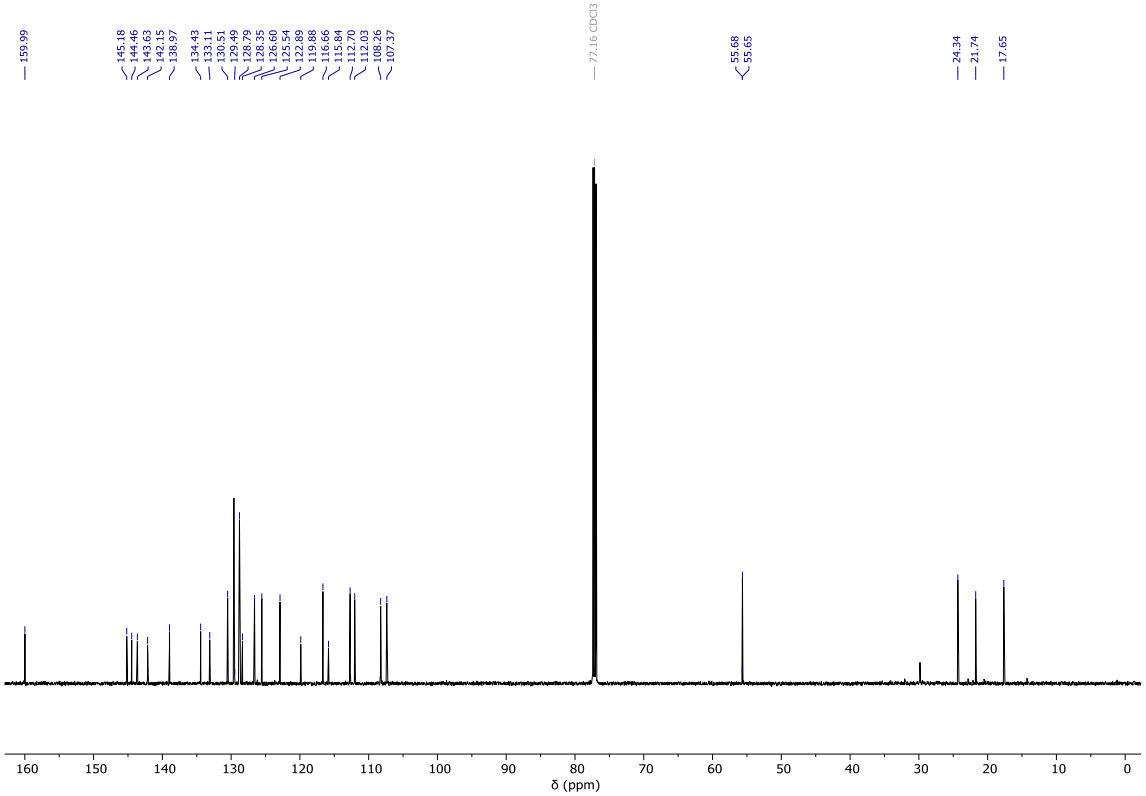
^{1}H-NMR spectrum of **34**. 600 MHz, $CDCl_3$



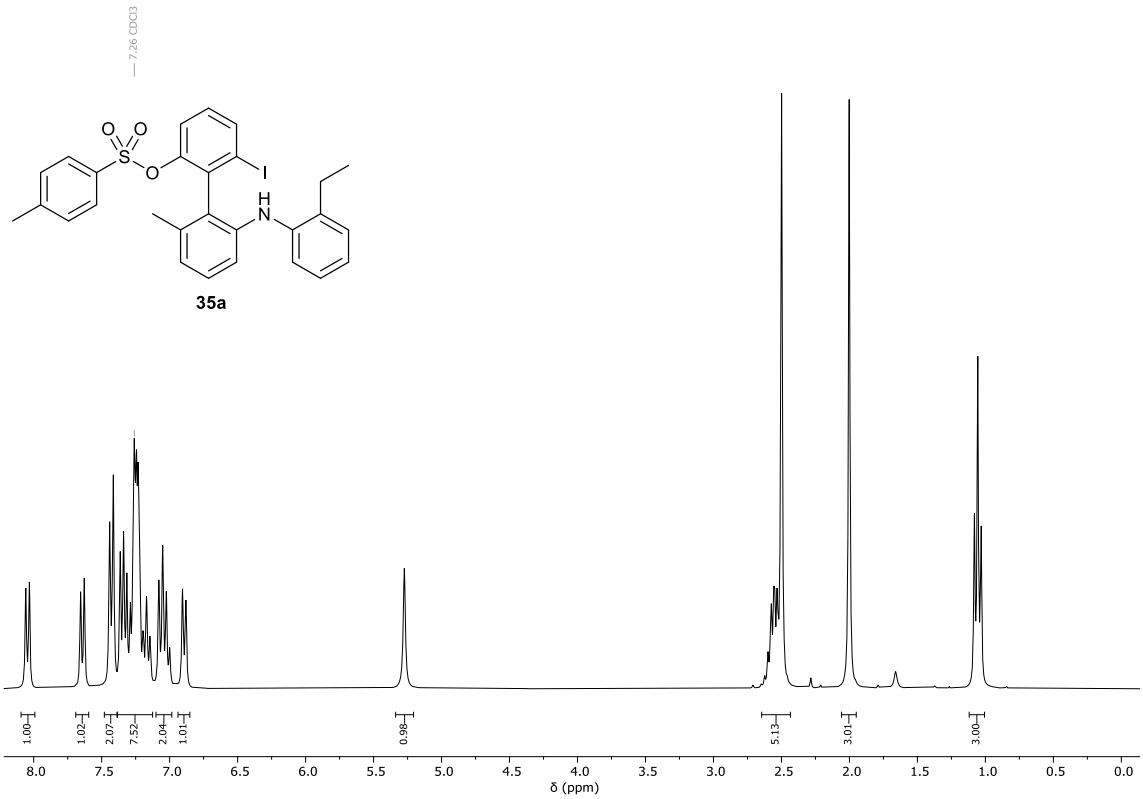
^{13}C-NMR spectrum of **34**. 75.5 MHz, $CDCl_3$



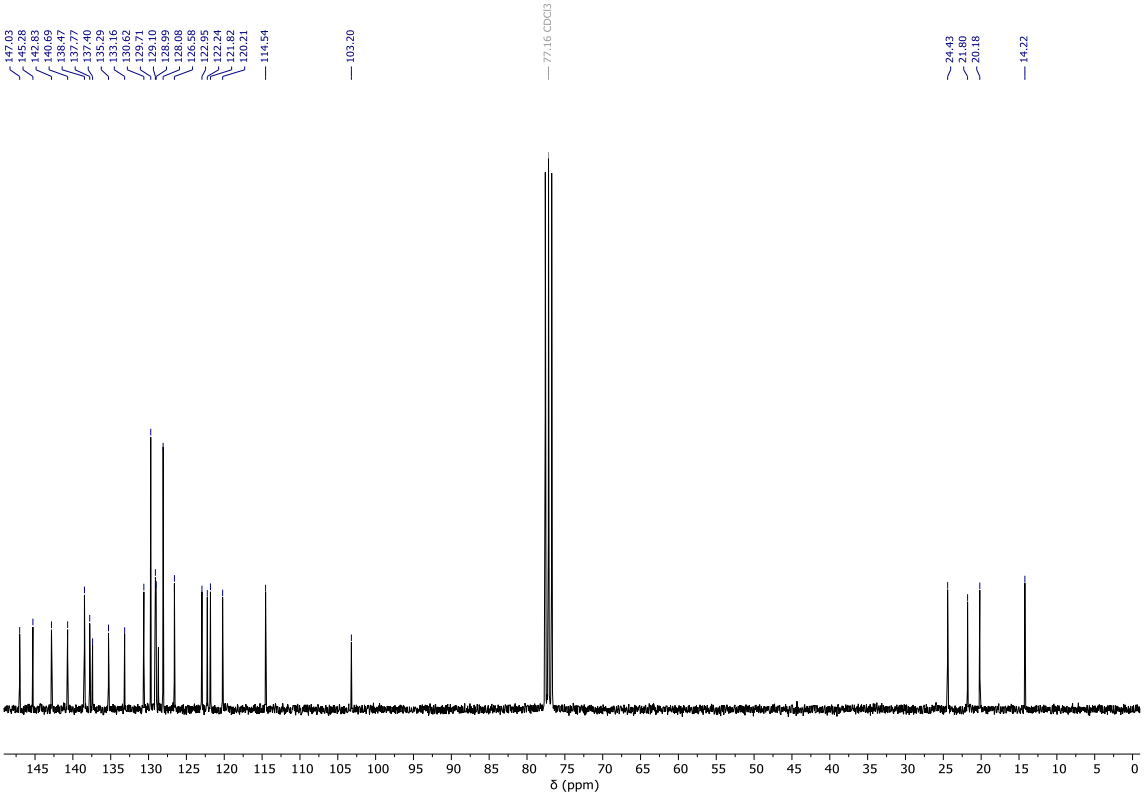
^{1}H-NMR spectrum of **13**. 600 MHz, $CDCl_3$



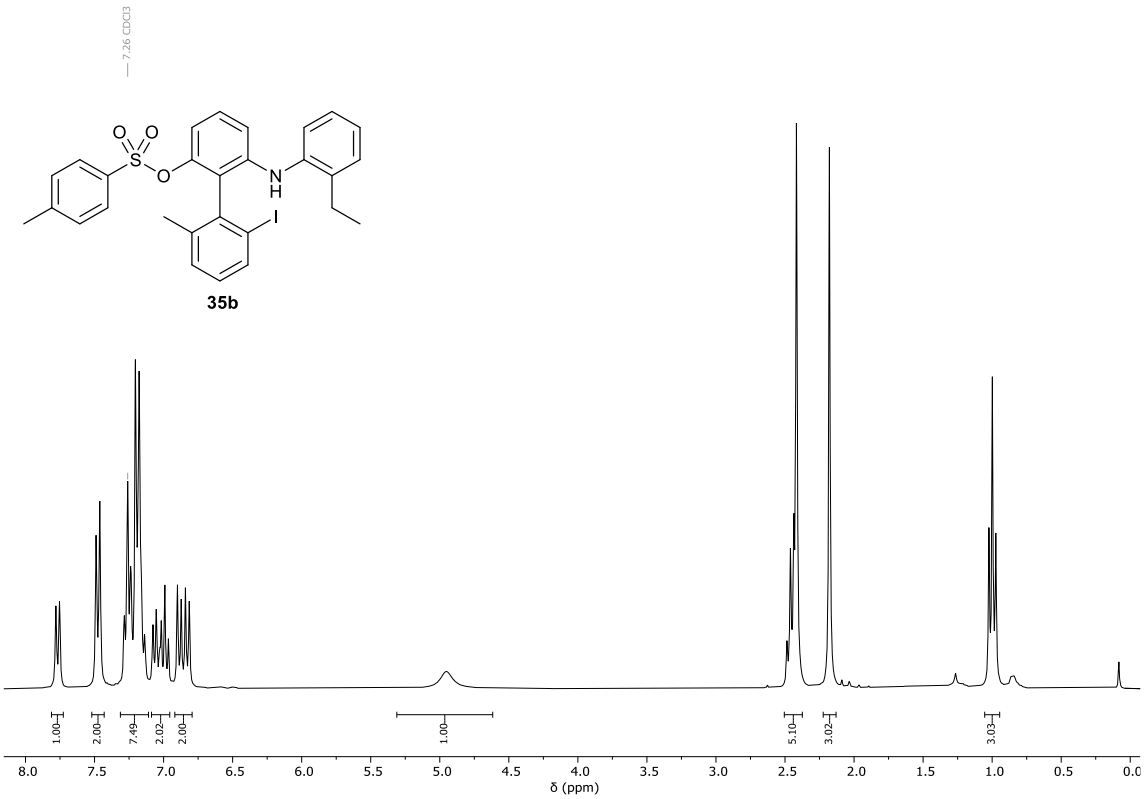
^{13}C-NMR spectrum of **13**. 151 MHz, $CDCl_3$



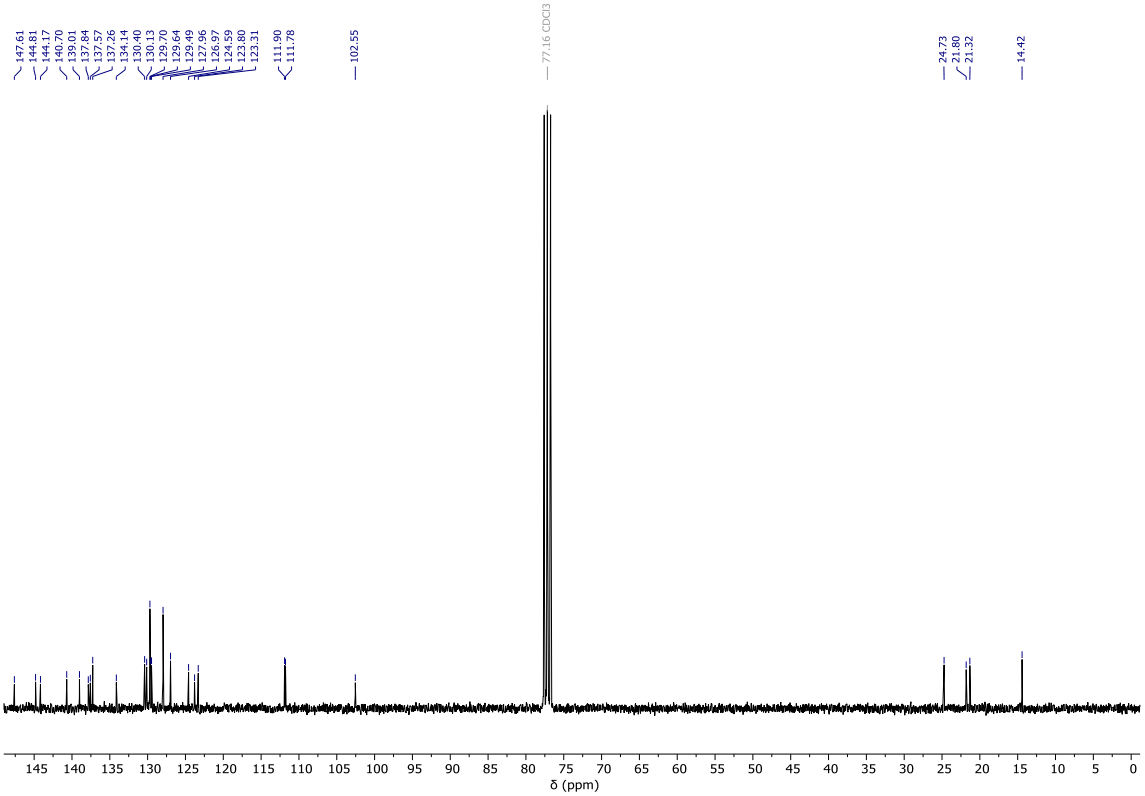
^{1}H-NMR spectrum of **35a**. 300 MHz, $CDCl_3$



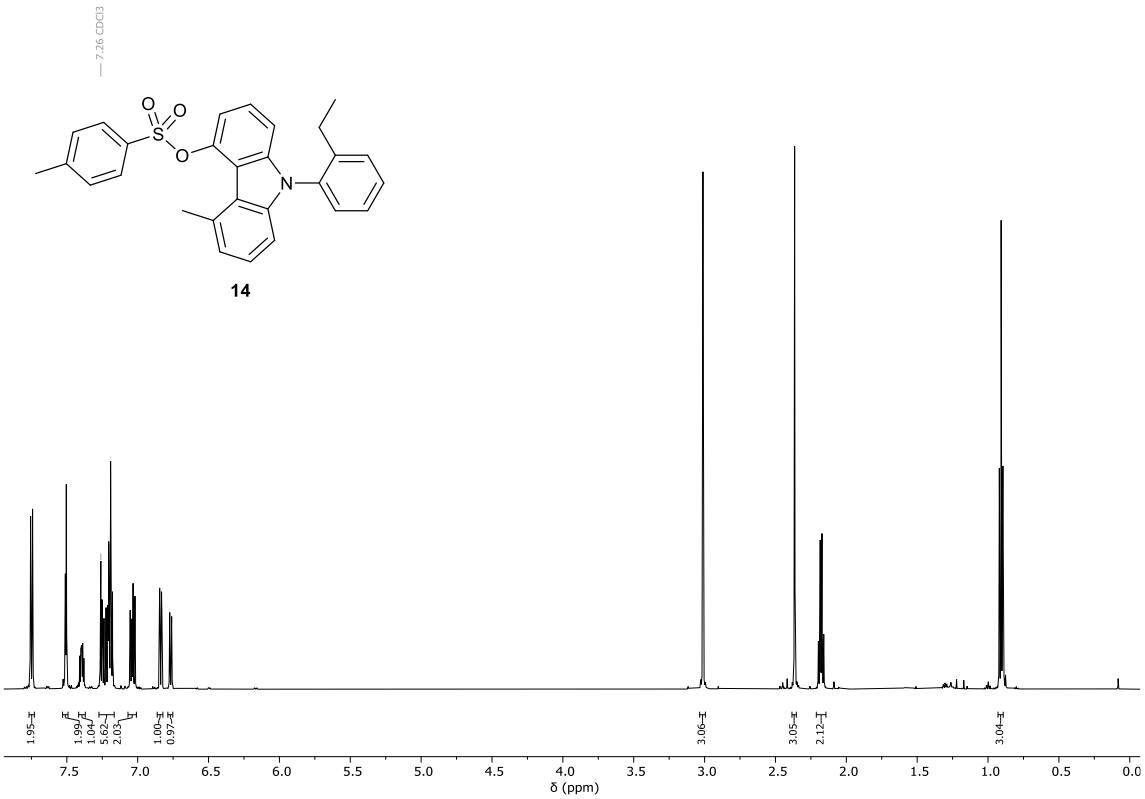
^{13}C-NMR spectrum of **35a**. 75.5 MHz, $CDCl_3$



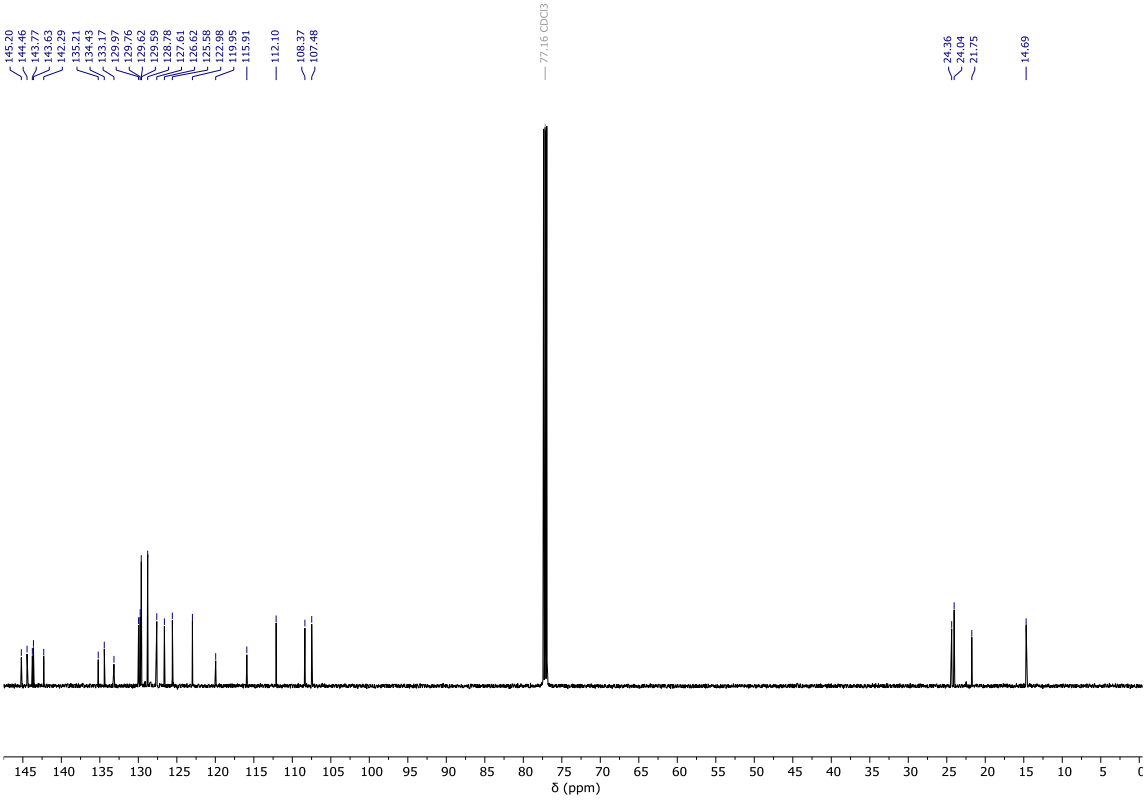
^{1}H-NMR spectrum of **35b**. 300 MHz, $CDCl_3$



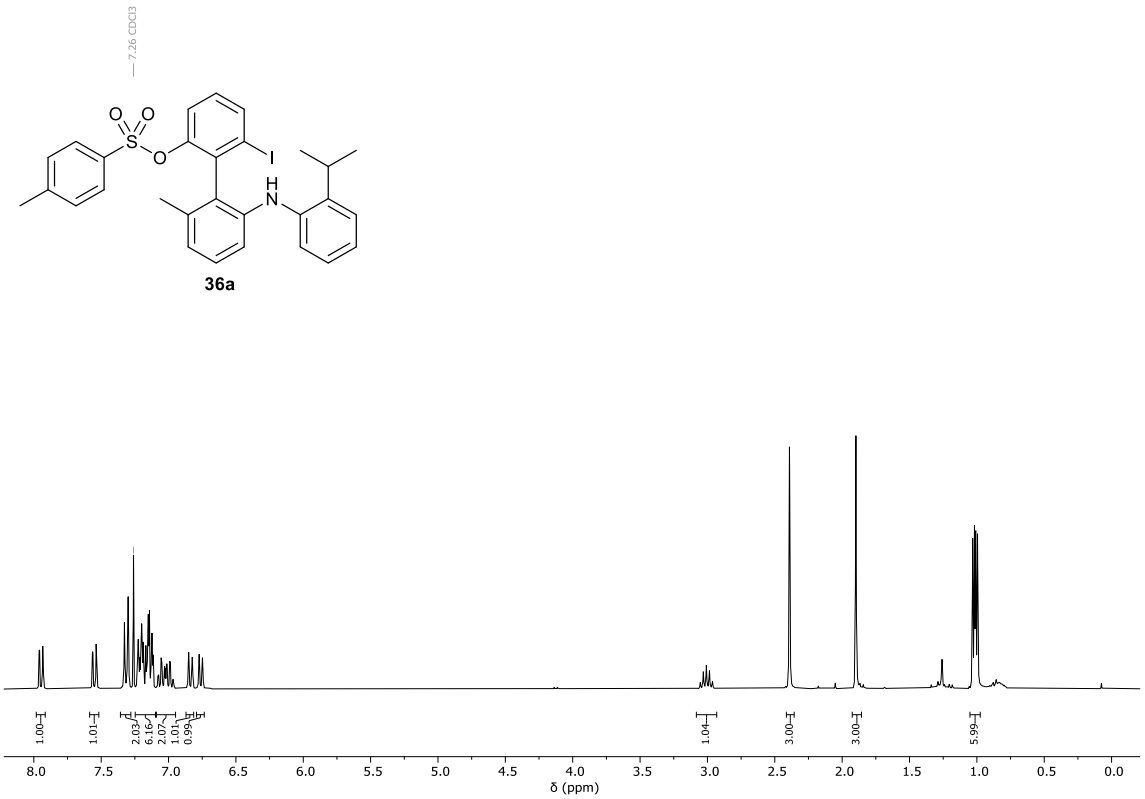
^{13}C-NMR spectrum of **35b**. 75.5 MHz, $CDCl_3$



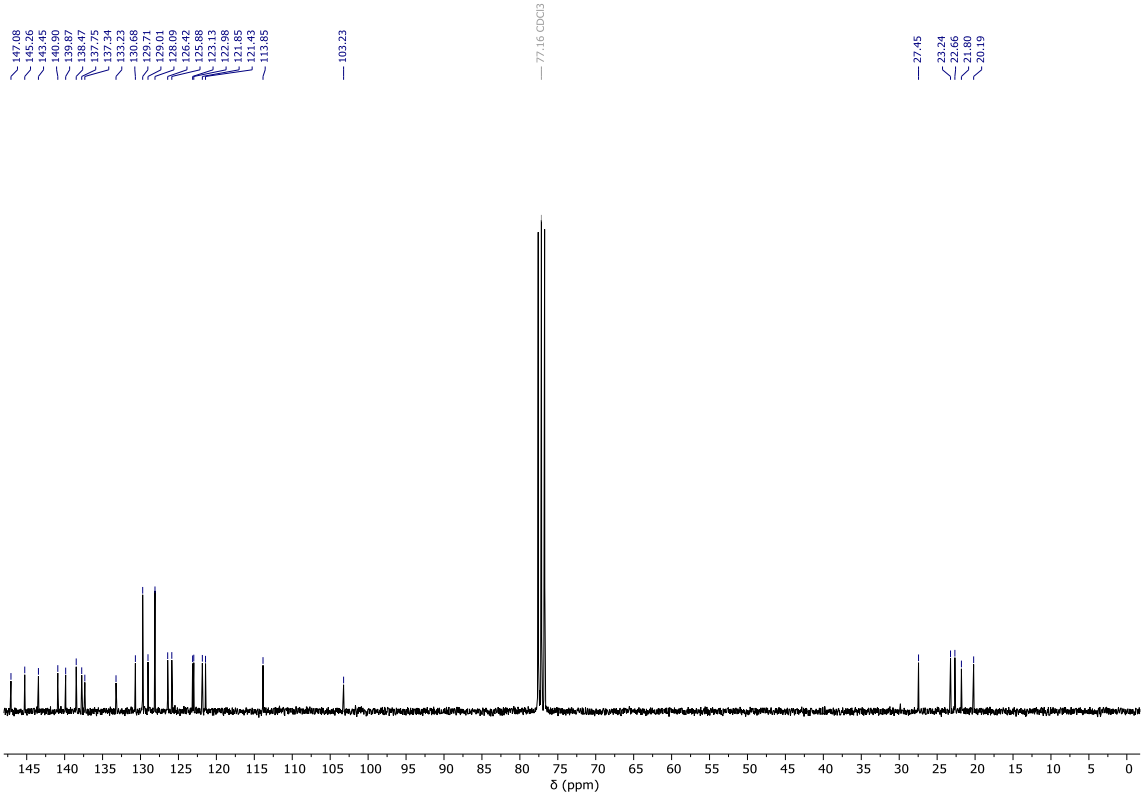
^{1}H-NMR spectrum of **14**. 600 MHz, $CDCl_3$



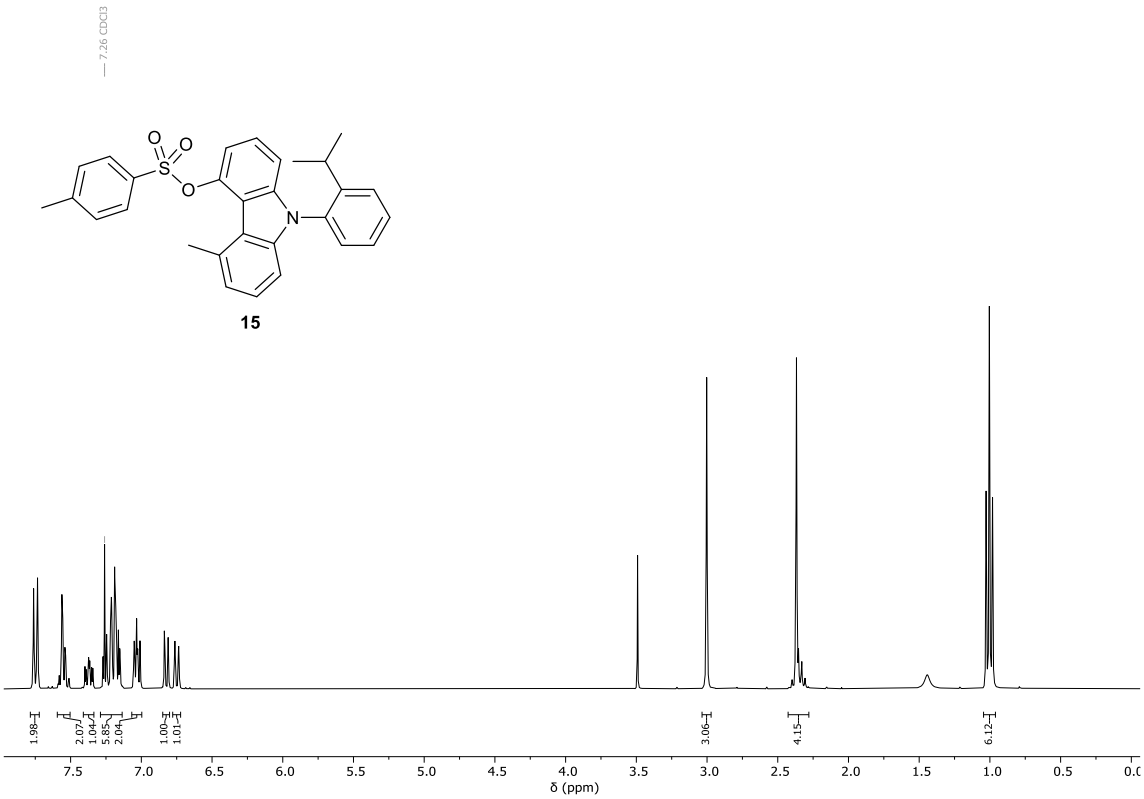
^{13}C-NMR spectrum of **14**. 151 MHz, $CDCl_3$



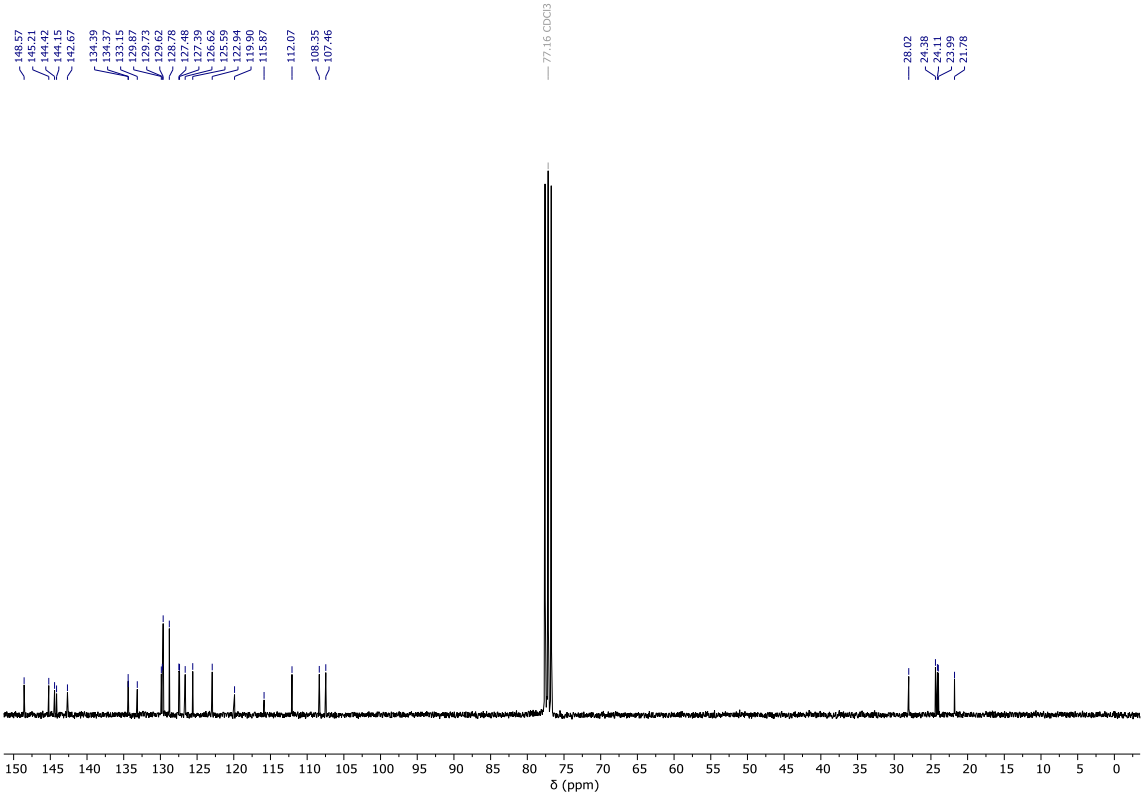
^{1}H-NMR spectrum of **36a**. 300 MHz, $CDCl_3$



^{13}C-NMR spectrum of **36a**. 75.5 MHz, $CDCl_3$

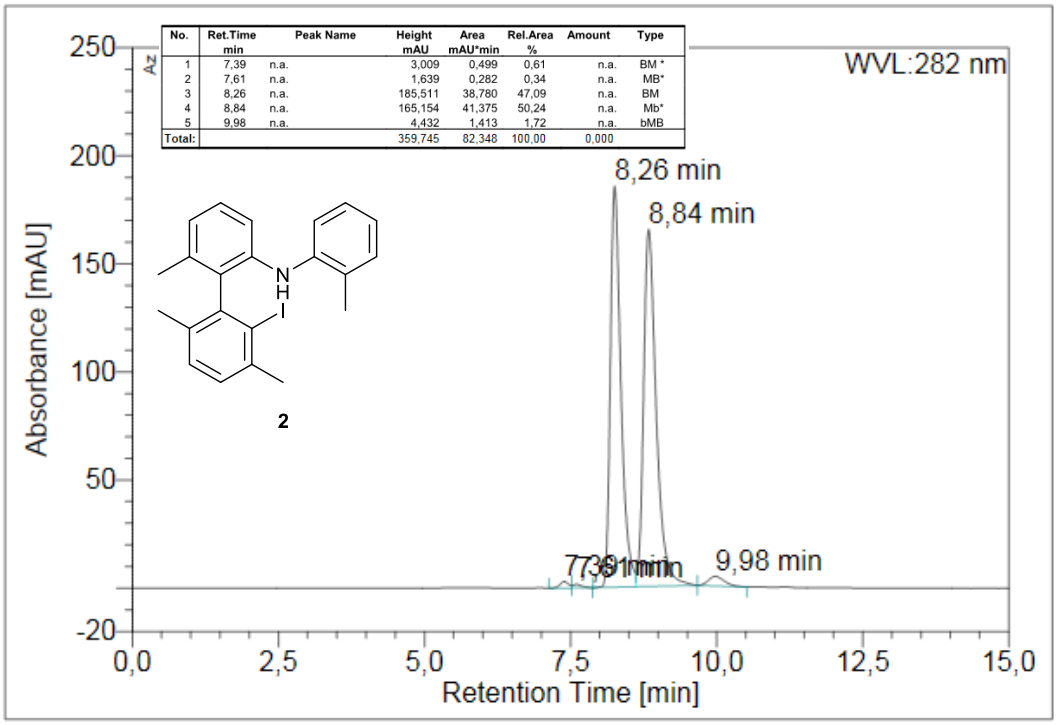


^{1}H-NMR spectrum of **15**. 300 MHz, $CDCl_3$

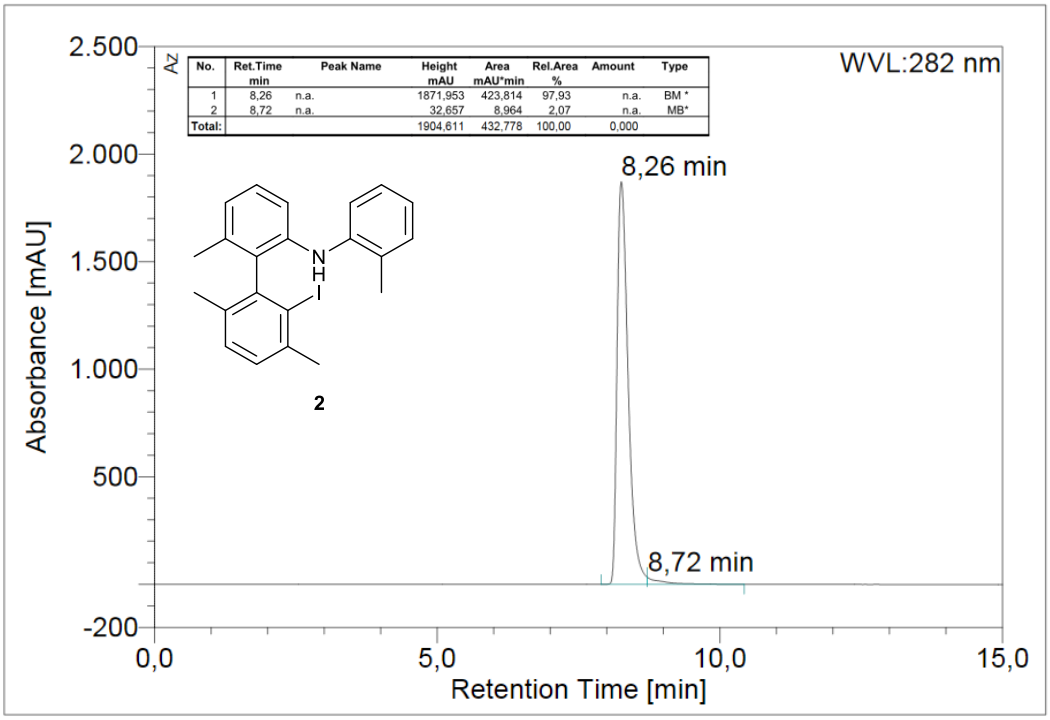


^{13}C-NMR spectrum of **15**. 75.5 MHz, $CDCl_3$

8. HPLC-traces

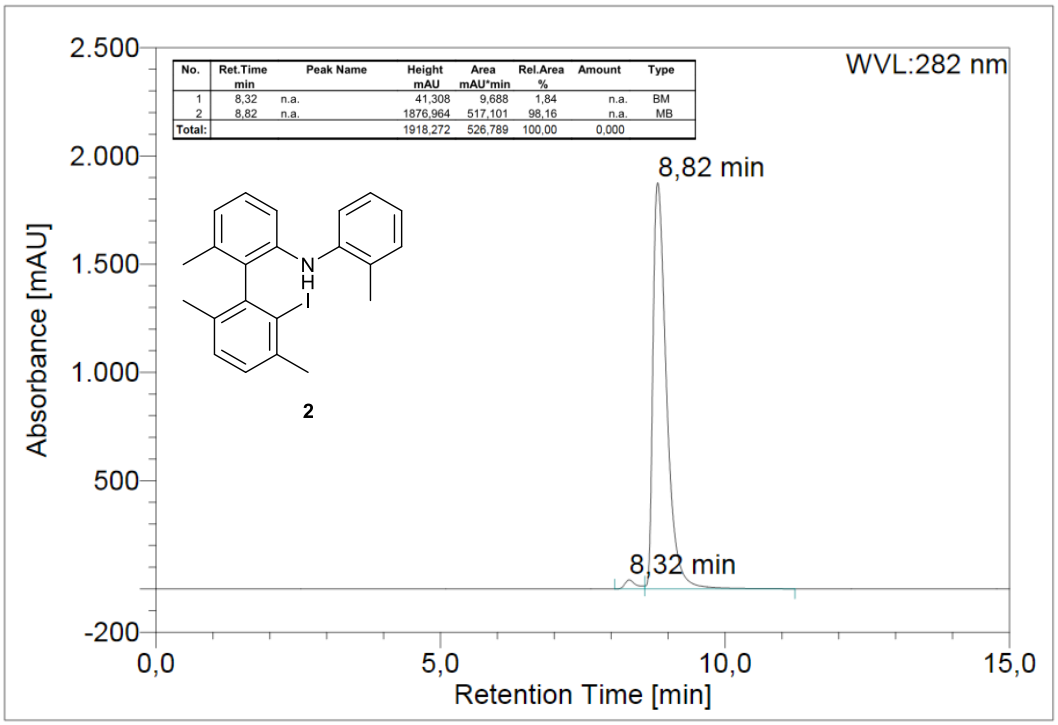


HPLC chromatogram of rac-**2**. Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 282 nm, *n*-heptane/*i*-PrOH: 99.6/0.4 (*v*/*v*), t_R(E1): 8.26 min, t_R(E2): 8.84 min



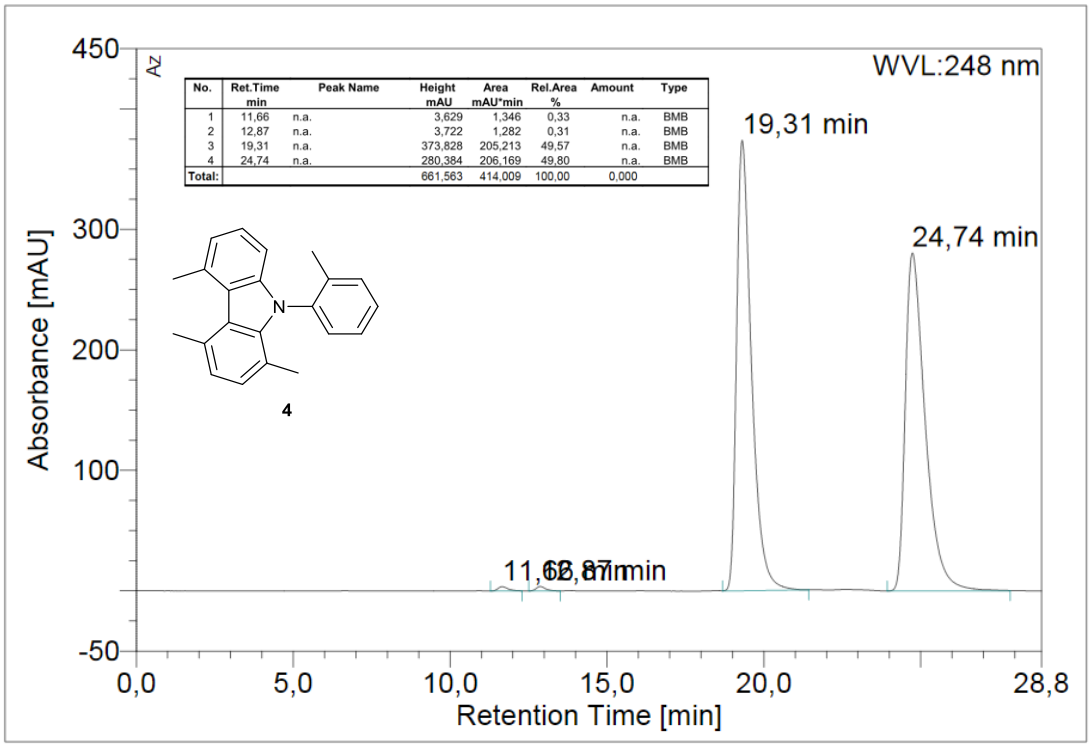
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8,26	n.a.	1871,953	423,814	97,93	n.a.	BM *
2	8,72	n.a.	32,657	8,964	2,07	n.a.	MB*
Total:			1904,611	432,778	100,00	0,000	

HPLC chromatogram of (+)-**2**. Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 282 nm, *n*-heptane/*i*-PrOH: 99.6/0.4 (*v*/*v*), t_R(E1): 8.26, >99% *ee*



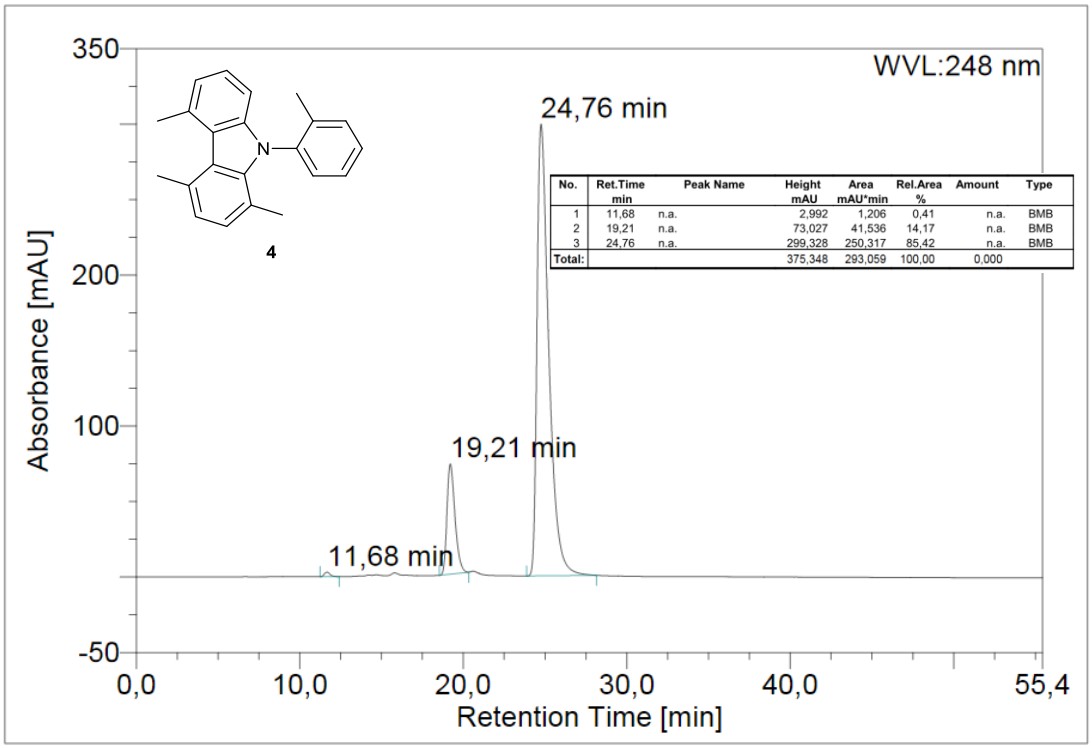
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	8,32	n.a.	41,308	9,688	1,84	n.a.	BM
2	8,82	n.a.	1876,964	517,101	98,16	n.a.	MB
Total:			1918,272	526,789	100,00	0,000	

HPLC chromatogram of (–)-**2**. Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 282 nm, *n*-heptane/*i*-PrOH: 99.6/0.4 (*v*/*v*), t_R(E1): 8.32 min, t_R(E2): 8.83 min, 96% ee



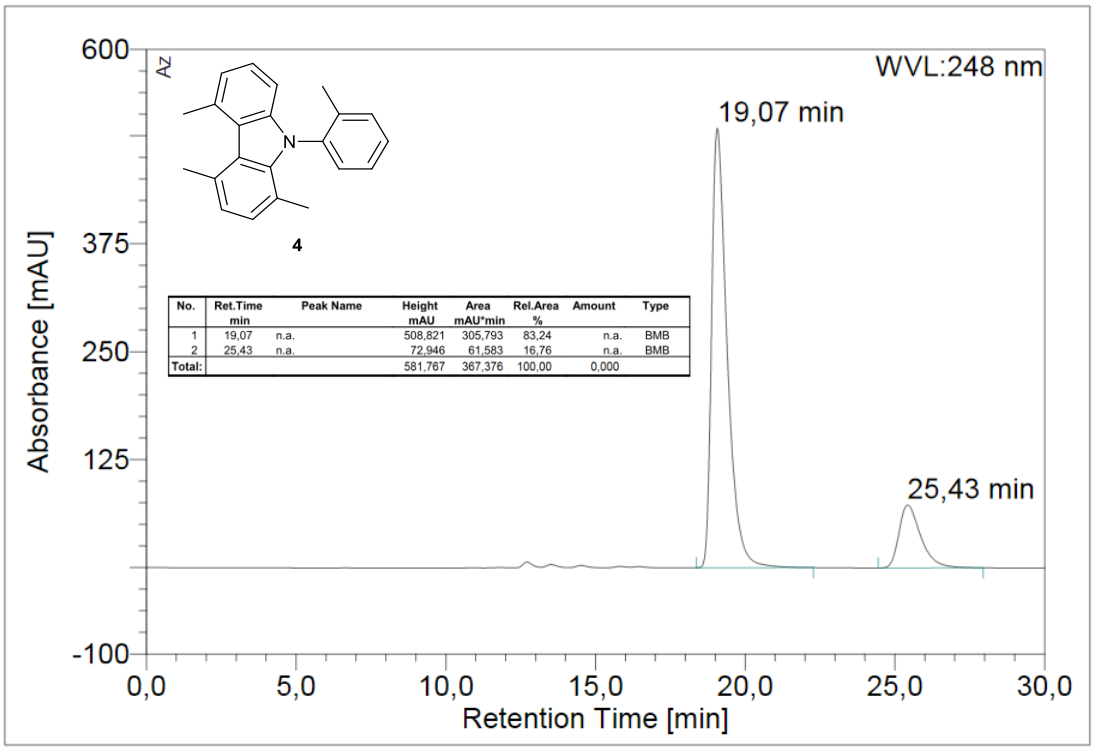
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11,66	n.a.	3,629	1,346	0,33	n.a.	BMB
2	12,87	n.a.	3,722	1,282	0,31	n.a.	BMB
3	19,31	n.a.	373,828	205,213	49,57	n.a.	BMB
4	24,74	n.a.	280,384	206,169	49,80	n.a.	BMB
Total:			661,563	414,009	100,00	0,000	

HPLC chromatogram of *rac*-**4**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 10 °C, 0.5 ml/min, 248 nm, *n*-heptane/*i*-PrOH: 99.8/0.2 (*v*/*v*), t_R(E1): 19.31 min, t_R(E2): 24.74 min



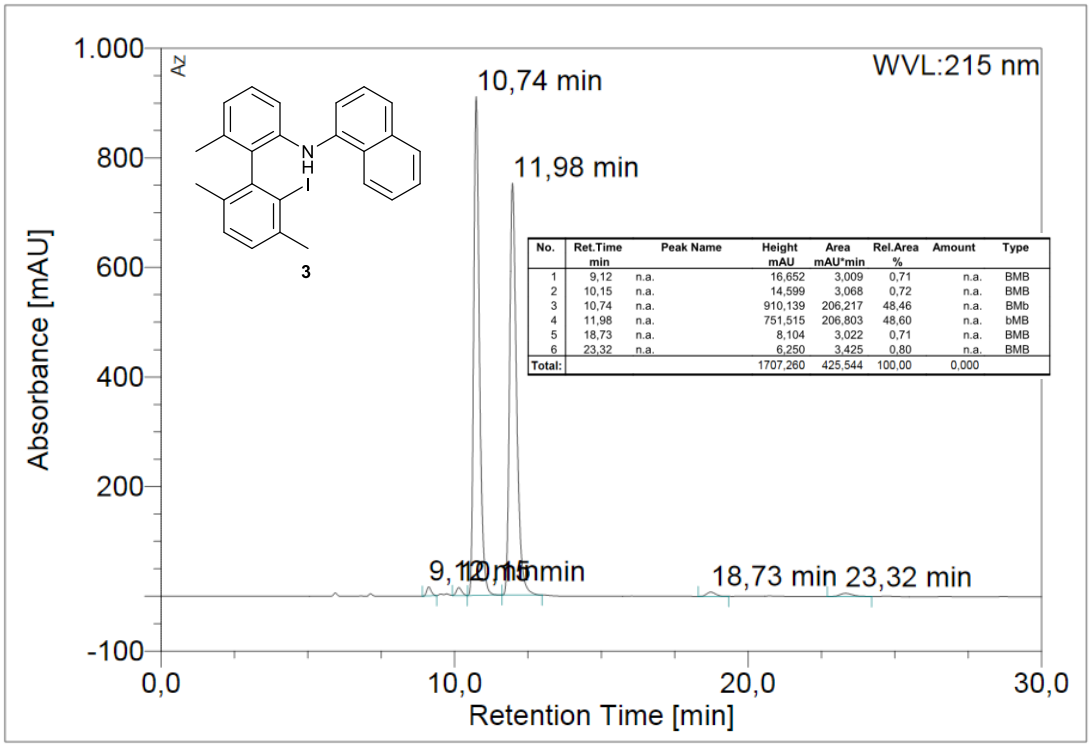
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	11,68	n.a.	2,992	1,206	0,41	n.a.	BMB
2	19,21	n.a.	73,027	41,536	14,17	n.a.	BMB
3	24,76	n.a.	299,328	250,317	85,42	n.a.	BMB
Total:			375,348	293,059	100,00	0,000	

HPLC chromatogram of (–)-**4**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 10 °C, 0.5 ml/min, 248 nm, *n*-heptane/*i*-PrOH: 99.8/0.2 (*v*/*v*), t_R(E1): 19.21 min, t_R(E2): 24.76 min, 61% *ee*



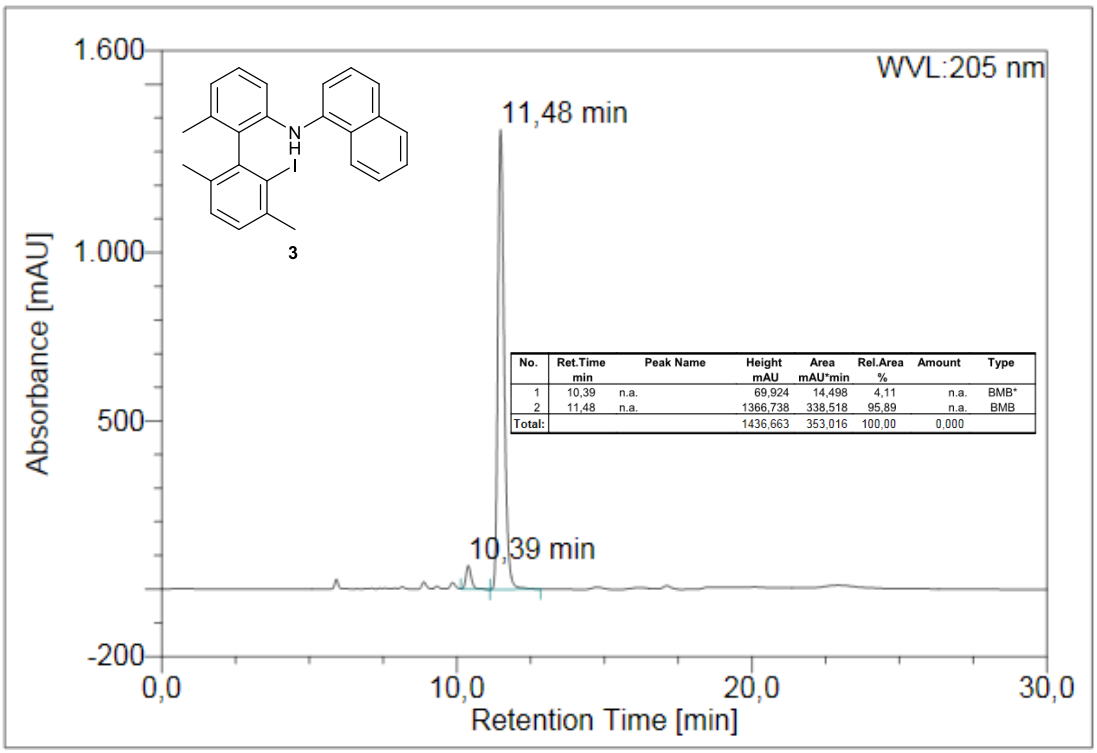
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	19,07	n.a.	508,821	305,793	83,24	n.a.	BMB
2	25,43	n.a.	72,946	61,583	16,76	n.a.	BMB
Total:			581,767	367,376	100,00	0,000	

HPLC chromatogram of (+)-**4**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 10 °C, 0.5 ml/min, 248 nm, *n*-heptane/*i*-PrOH: 99.8/0.2 (*v*/*v*), t_R(E1): 19.07 min, t_R(E2): 25.43 min, 67% *ee*



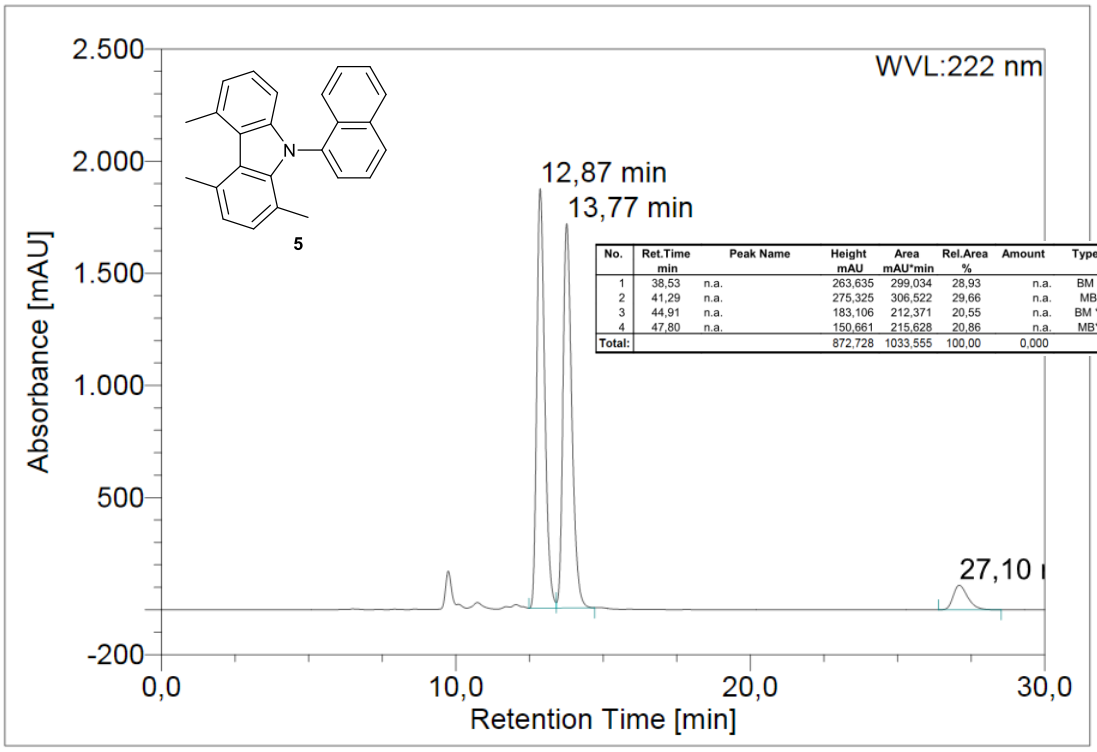
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	9,12	n.a.	16,652	3,009	0,71	n.a.	BMB
2	10,15	n.a.	14,599	3,068	0,72	n.a.	BMB
3	10,74	n.a.	910,139	206,217	48,46	n.a.	BMb
4	11,98	n.a.	751,515	206,803	48,60	n.a.	bMB
5	18,73	n.a.	8,104	3,022	0,71	n.a.	BMB
6	23,32	n.a.	6,250	3,425	0,80	n.a.	BMB
Total:			1707,260	425,544	100,00	0,000	

HPLC chromatogram of *rac*-**3**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 10 °C, 0.5 ml/min, 282 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 10.74 min, t_R(E1): 11.98 min



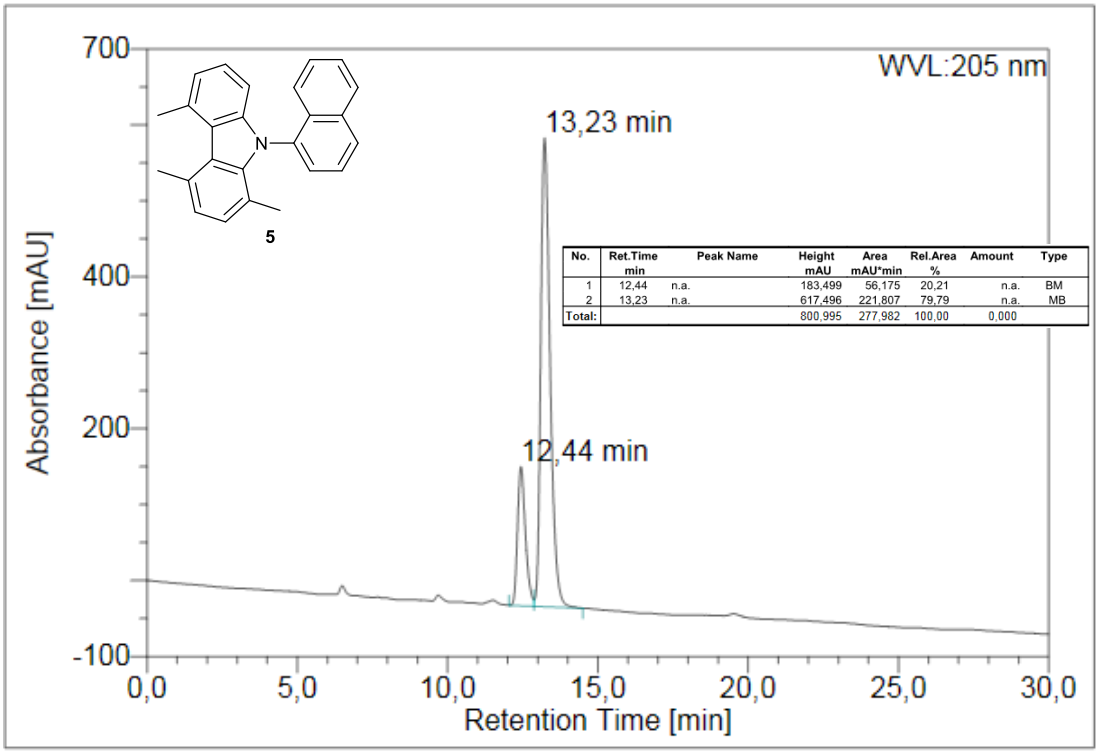
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,39	n.a.	69,924	14,498	4,11	n.a.	BMB*
2	11,48	n.a.	1366,738	338,518	95,89	n.a.	BMB
Total:			1436,663	353,016	100,00	0,000	

HPLC chromatogram of (–)-**3**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 10 °C, 0.5 ml/min, 282 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 10.39 min, t_R(E1): 11.48 min, >92% *ee*

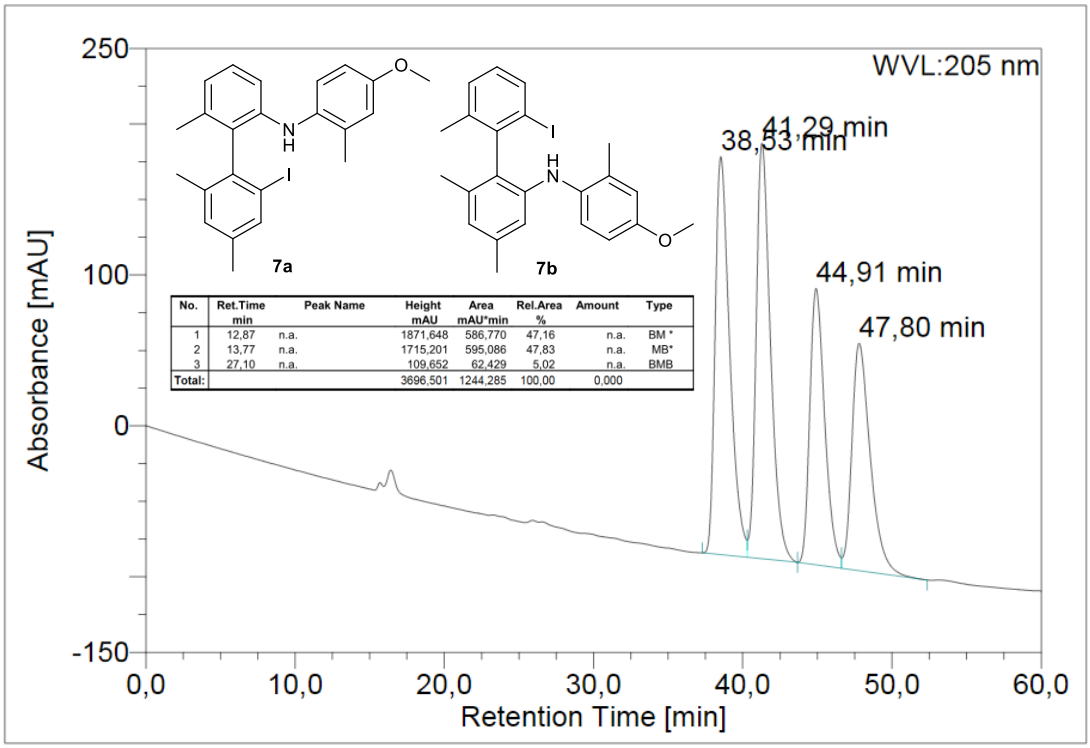


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	38,53	n.a.	263,635	299,034	28,93	n.a.	BM
2	41,29	n.a.	275,325	306,522	29,66	n.a.	MB
3	44,91	n.a.	183,106	212,371	20,55	n.a.	BM *
4	47,80	n.a.	150,661	215,628	20,86	n.a.	MB*
Total:			872,728	1033,555	100,00	0,000	

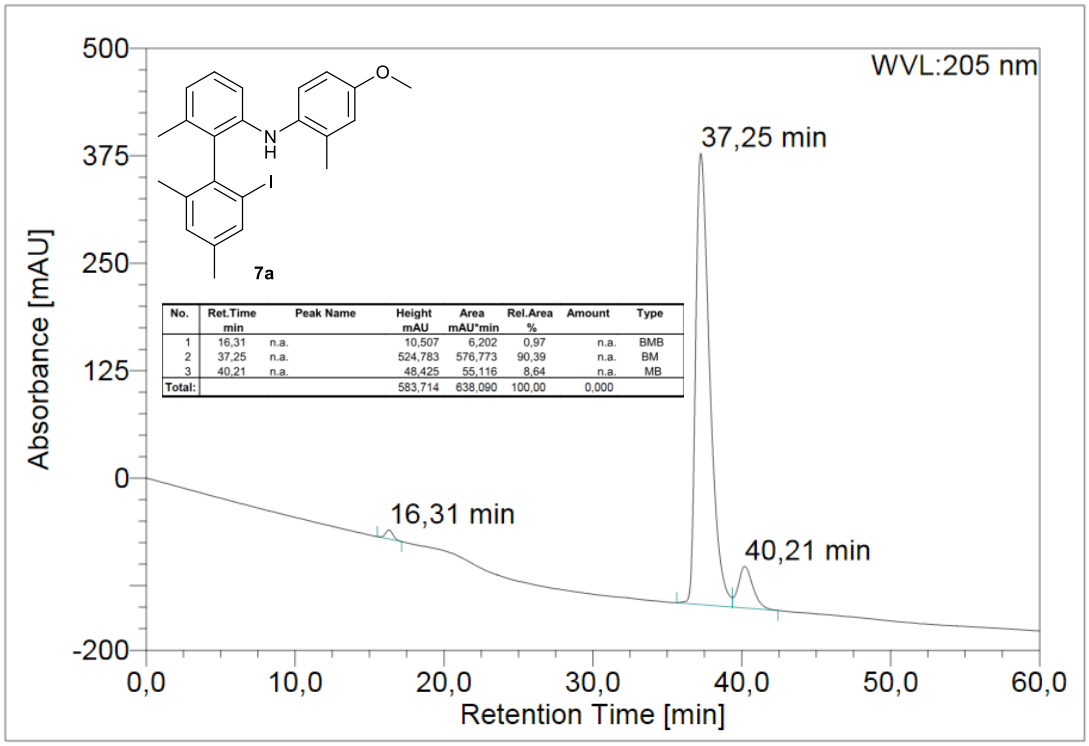
HPLC chromatogram of *rac*-**5**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.5 ml/min, 222 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 12.87 min, t_R(E2): 13.77 min



HPLC chromatogram of (–)-**5**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 12.44 min, t_R(E2): 13.23 min, 60% *ee*

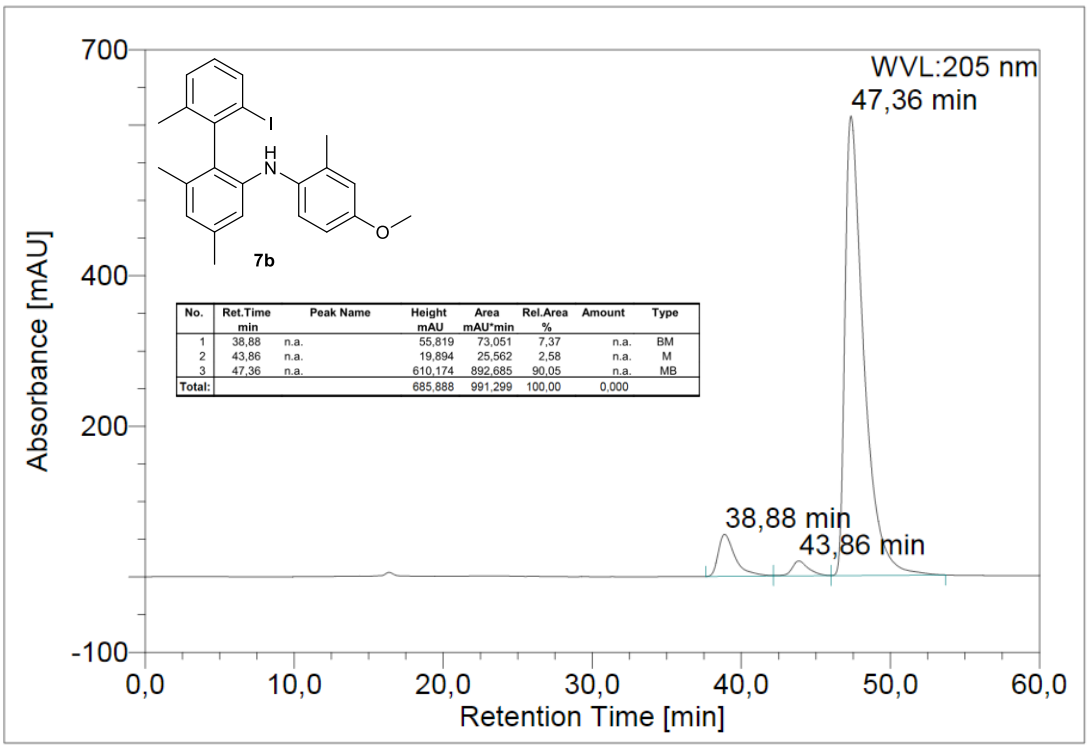


HPLC chromatogram of *rac*-**7a** and *rac*-**7b**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.2 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.8/0.2 (*v*/*v*), t_R(E1): 38.53 min, t_R(E2): 41.29 min, t_R(E3): 44.91 min, t_R(E4): 47.80 min



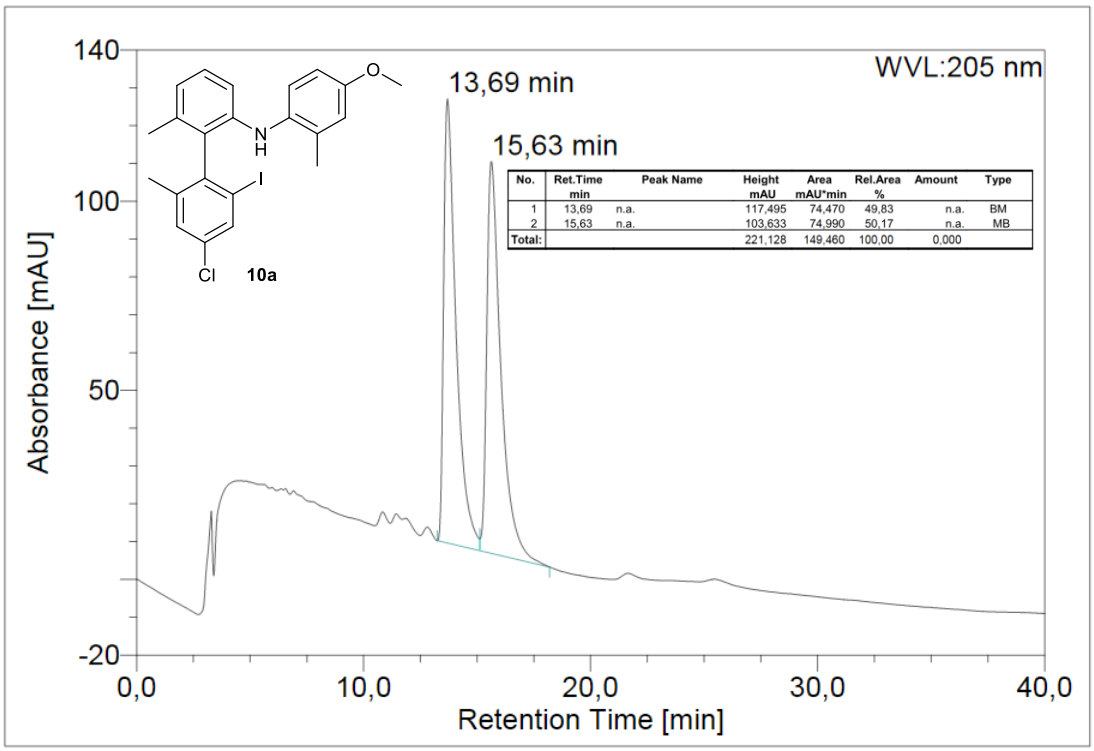
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16,31	n.a.		10,507	6,202	0,97	n.a.	BMB
2	37,25	n.a.		524,783	576,773	90,39	n.a.	BM
3	40,21	n.a.		48,425	55,116	8,64	n.a.	MB
Total:				583,714	638,090	100,00	0,000	

HPLC chromatogram of (–)-**7a**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.2 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.8/0.2 (*v*/*v*), t_R(E1): 37.25 min, t_R(E2): 40.21 min, 83% *ee*



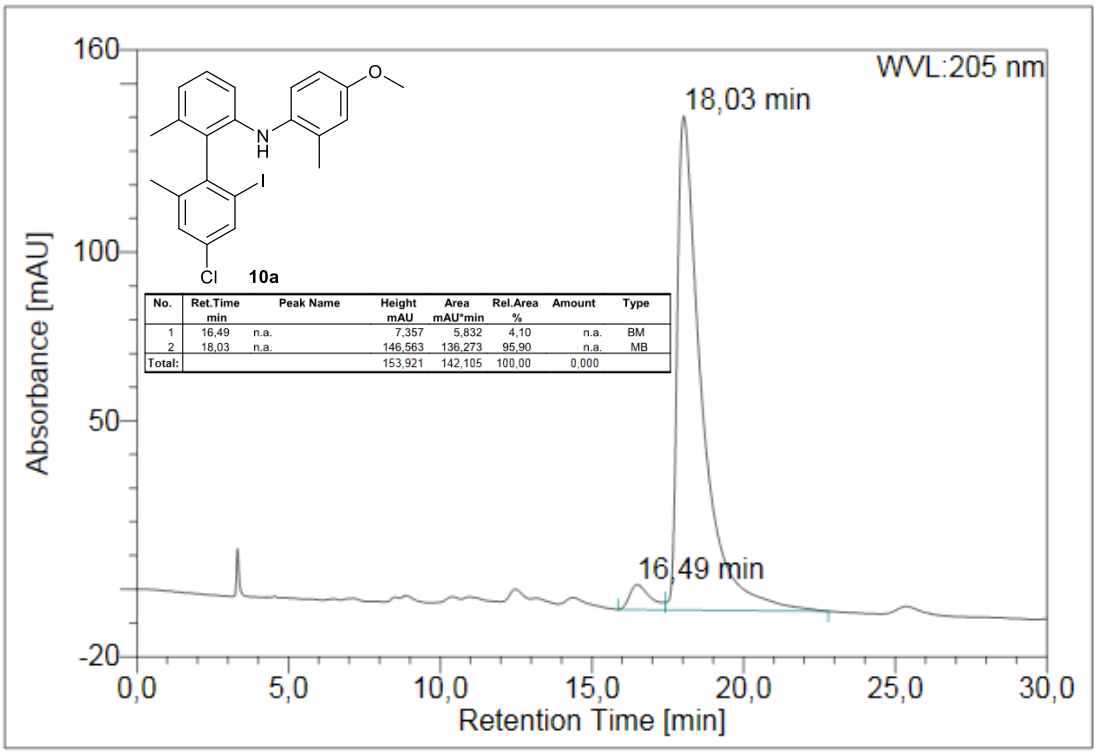
No.	Ret.Time min		Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	38,88	n.a.		55,819	73,051	7,37	n.a.	BM
2	43,86	n.a.		19,894	25,562	2,58	n.a.	M
3	47,36	n.a.		610,174	892,685	90,05	n.a.	MB
Total:				685,888	991,299	100,00	0,000	

HPLC chromatogram of (–)-**7b**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.2 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.8/0.2 (*v*/*v*), t_R(E1): 43.86 min, t_R(E2): 47.36 min, 94% *ee*, regioisomeric ratio: 92.6/7.4



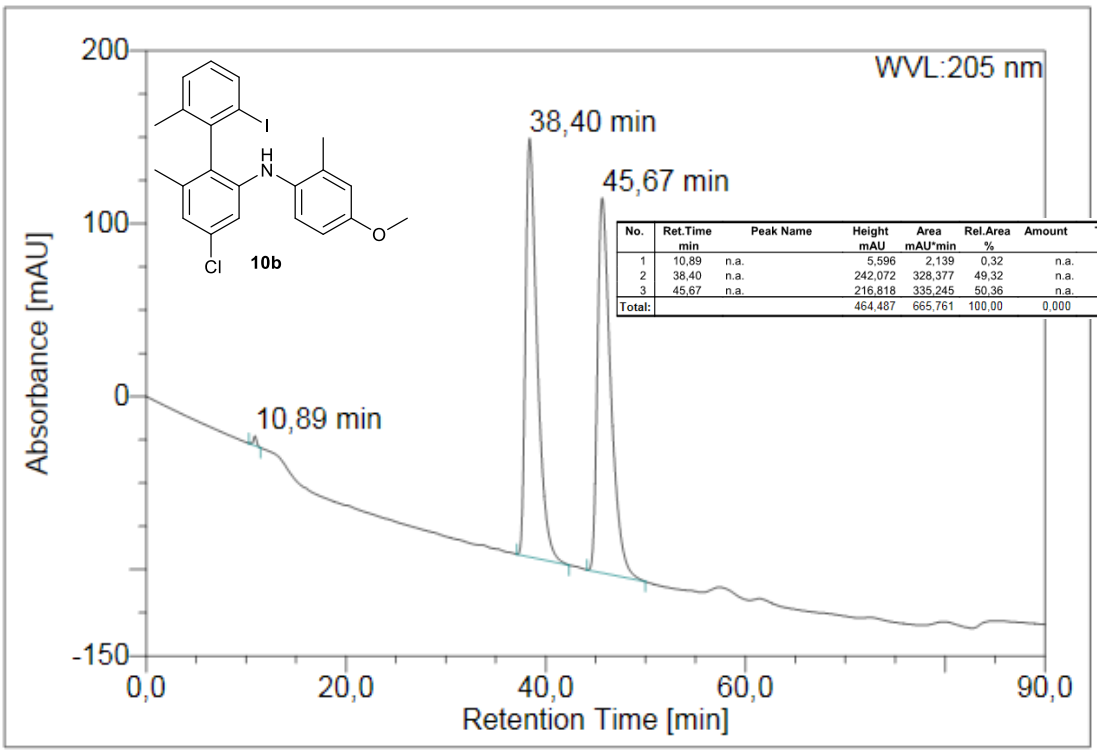
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13,69	n.a.	117,495	74,470	49,83	n.a.	BM
2	15,63	n.a.	103,633	74,990	50,17	n.a.	MB
Total:			221,128	149,460	100,00	0,000	

HPLC chromatogram of *rac*-**10a**, Chiralpak® IB (Daicel) 250 × 4.6 mm, 10 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.9/0.1 (*v*/*v*), t_R(E1): 13.69 min, t_R(E2): 15.63 min



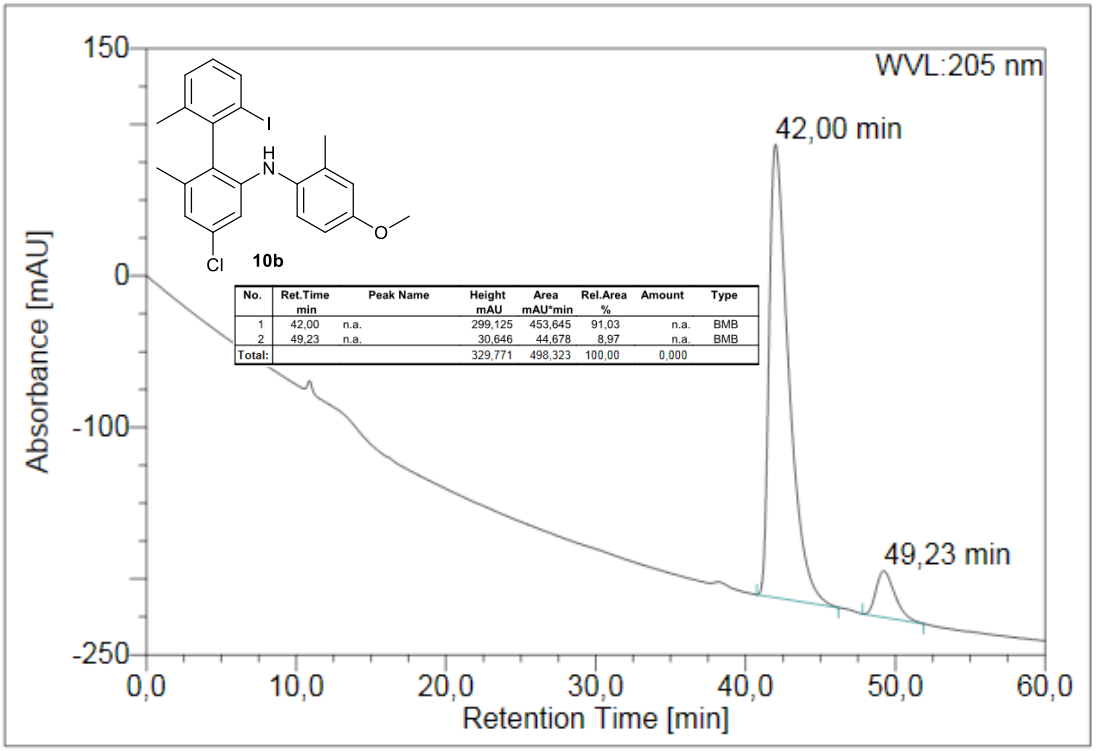
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16,49	n.a.	7,357	5,832	4,10	n.a.	BM
2	18,03	n.a.	146,563	136,273	95,90	n.a.	MB
Total:			153,921	142,105	100,00	0,000	

HPLC chromatogram of (–)-**10a**, Chiralpak® IB (Daicel) 250 × 4.6 mm, 10 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.9/0.1 (*v*/*v*), t_R(E1): 16.49 min, t_R(E2): 18.03 min, 92% *ee*



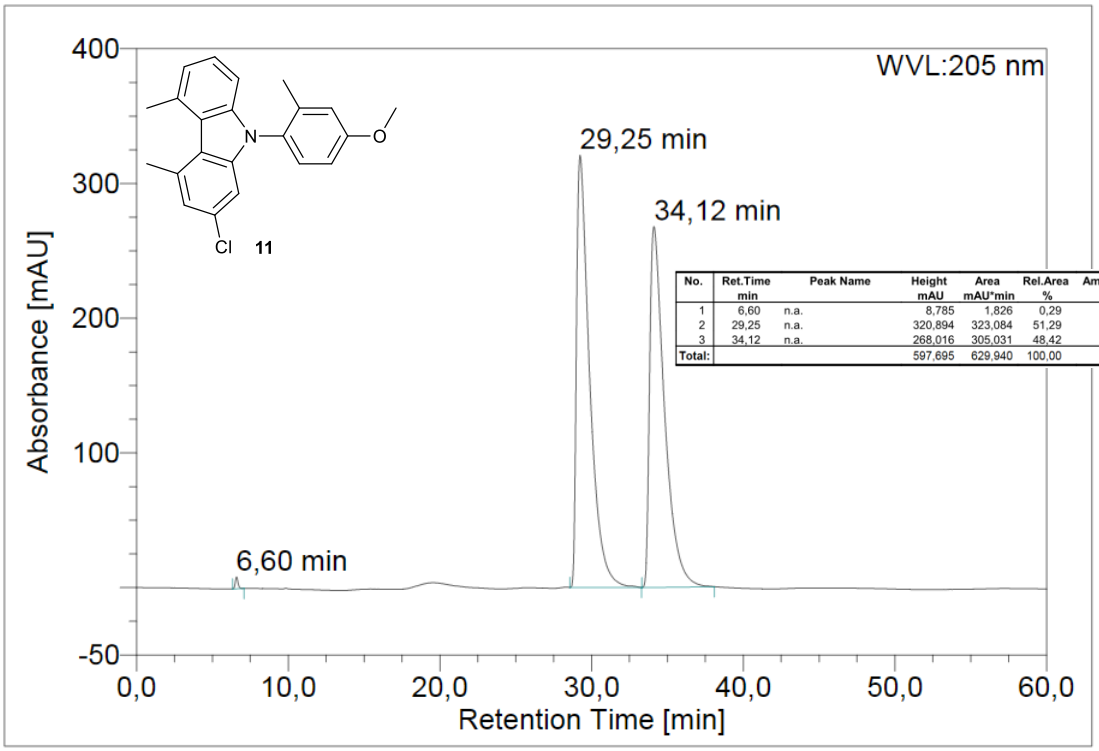
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,89	n.a.	5,596	2,139	0,32	n.a.	BMB
2	38,40	n.a.	242,072	328,377	49,32	n.a.	BMB
3	45,67	n.a.	216,818	335,245	50,36	n.a.	BMB
Total:			464,487	665,761	100,00	0,000	

HPLC chromatogram of *rac*-**10b**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.3 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.9/0.1 (*v*/*v*), t_R(E1): 38.40 min, t_R(E2): 45.67 min



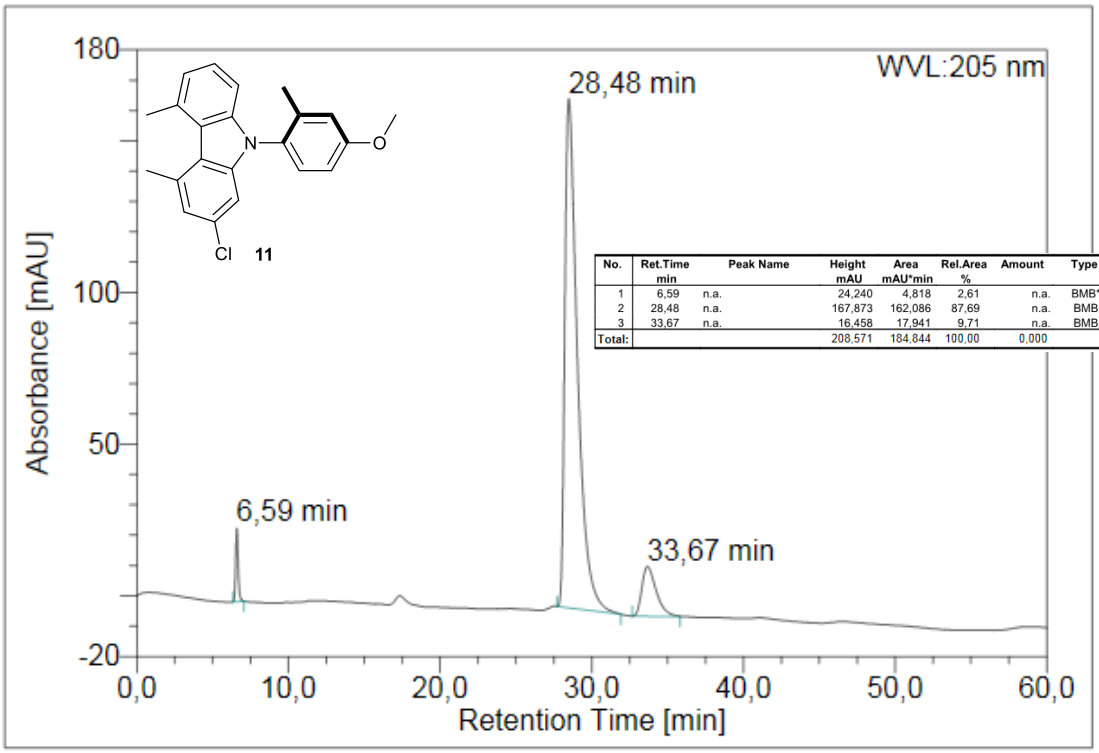
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	42,00	n.a.	299,125	453,645	91,03	n.a.	BMB
2	49,23	n.a.	30,646	44,678	8,97	n.a.	BMB
Total:			329,771	498,323	100,00	0,000	

HPLC chromatogram of (–)-**10b**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.3 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.9/0.1 (*v*/*v*), t_R(E1): 42.00 min, t_R(E2): 49.23 min, 82% *ee*



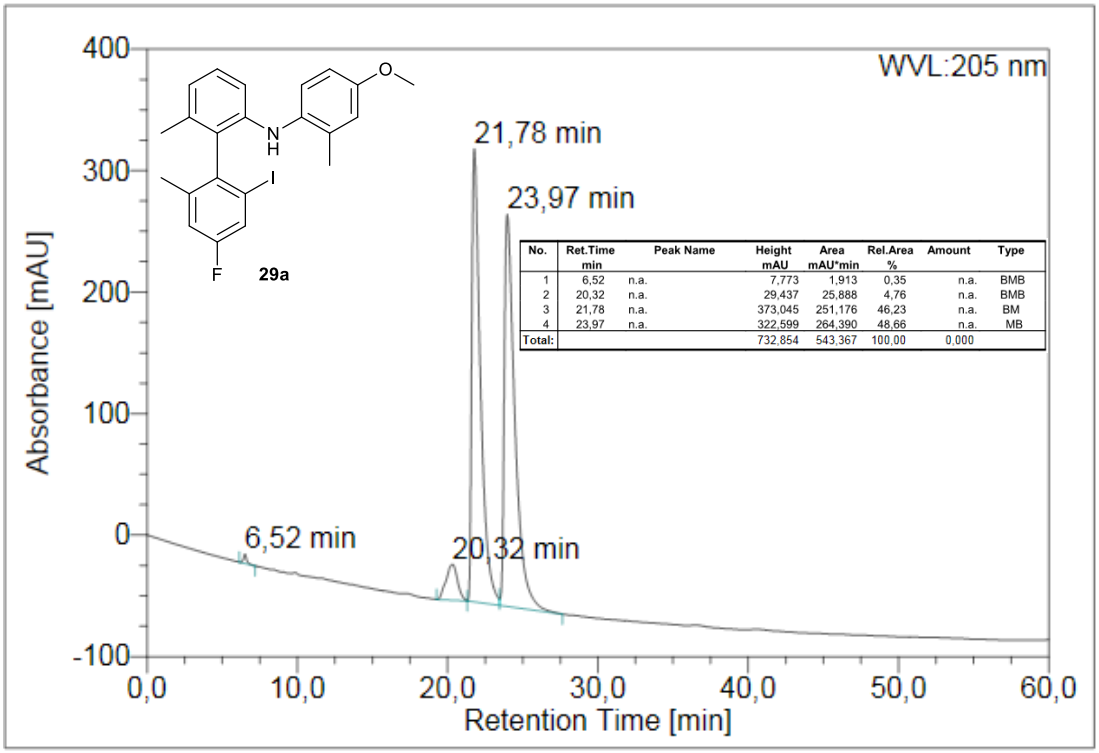
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6,60	n.a.	8,785	1,826	0,29	n.a.	BMB
2	29,25	n.a.	320,894	323,084	51,29	n.a.	BMB
3	34,12	n.a.	268,016	305,031	48,42	n.a.	BMB
Total:			597,695	629,940	100,00	0,000	

HPLC chromatogram of *rac*-**11**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.9/0.1 (*v*/*v*), t_R(E1): 29.25 min, t_R(E2): 34.12 min



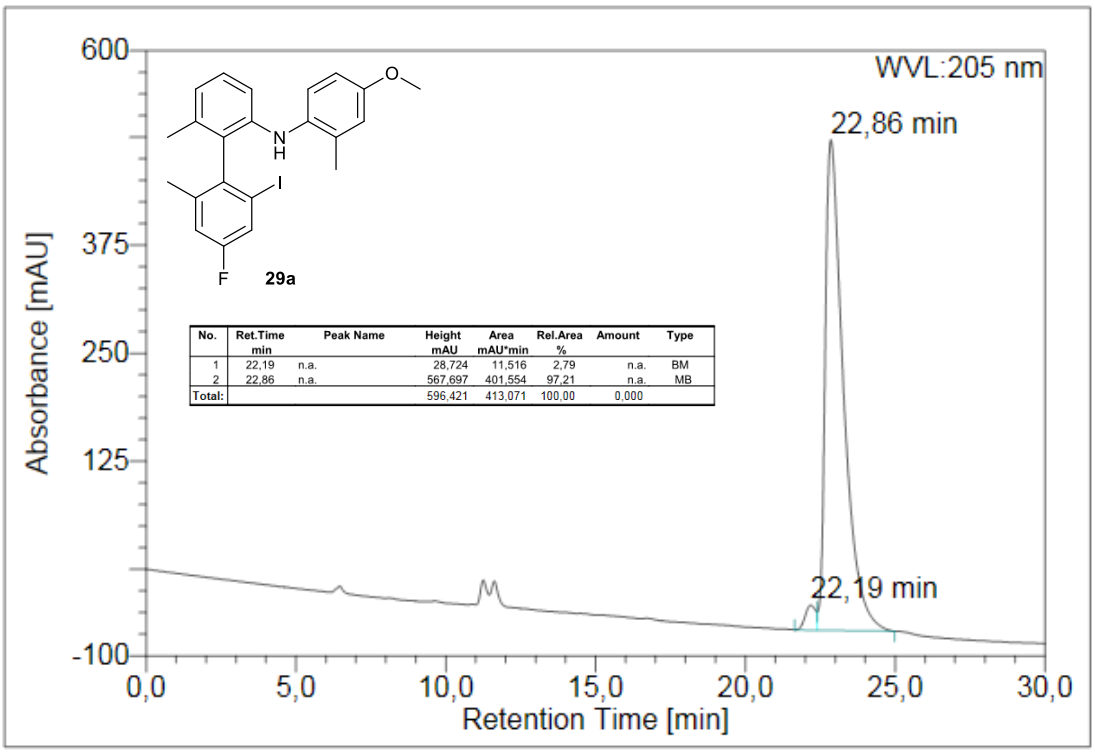
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6,59	n.a.	24,240	4,818	2,61	n.a.	BMB*
2	28,48	n.a.	167,873	162,086	87,69	n.a.	BMB
3	33,67	n.a.	16,458	17,941	9,71	n.a.	BMB
Total:			208,571	184,844	100,00	0,000	

HPLC chromatogram of (S_a)-**11**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.9/0.1 (*v*/*v*), t_R(E1): 28.48 min, t_R(E2): 33.67 min, 80% *ee*



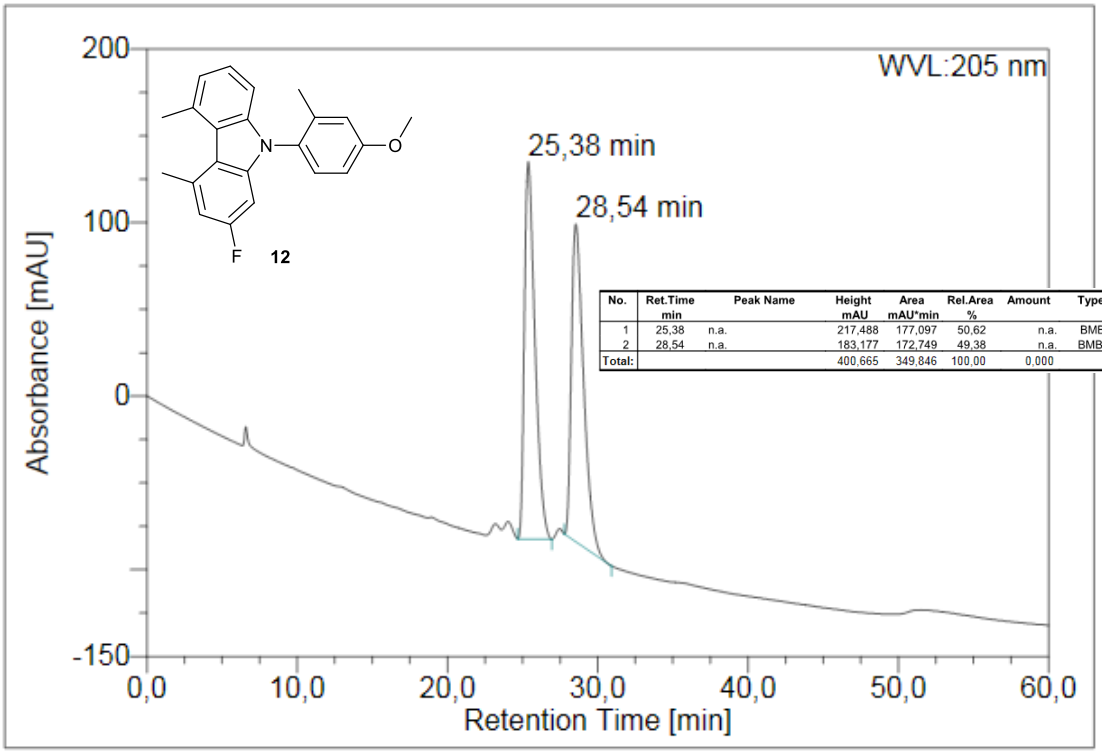
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	6,52	n.a.	7,773	1,913	0,35	n.a.	BMB
2	20,32	n.a.	29,437	25,888	4,76	n.a.	BMB
3	21,78	n.a.	373,045	251,176	46,23	n.a.	BM
4	23,97	n.a.	322,599	264,390	48,66	n.a.	MB
Total:			732,854	543,367	100,00	0,000	

HPLC chromatogram of *rac*-**29a**, Chiralpak® IB (Daicel) 250 × 4.6 mm, 20 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.99/0.01 (*v*/*v*), t_R(E1): 21.78 min, t_R(E2): 23.97 min



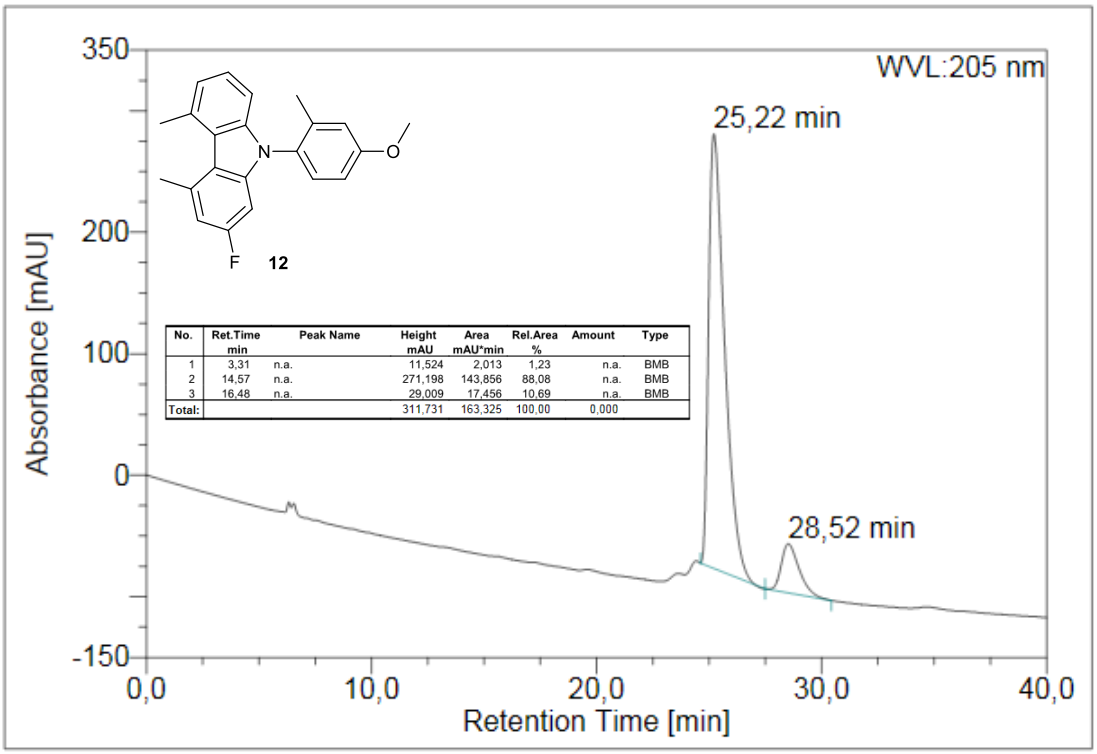
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	22,19	n.a.	28,724	11,516	2,79	n.a.	BM
2	22,86	n.a.	567,697	401,554	97,21	n.a.	MB
Total:			596,421	413,071	100,00	0,000	

HPLC chromatogram of (–)-**29a**, Chiralpak® IB (Daicel) 250 × 4.6 mm, 20 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.99/0.01 (*v*/*v*), t_R(E1): 22.19 min, t_R(E2): 22.86 min



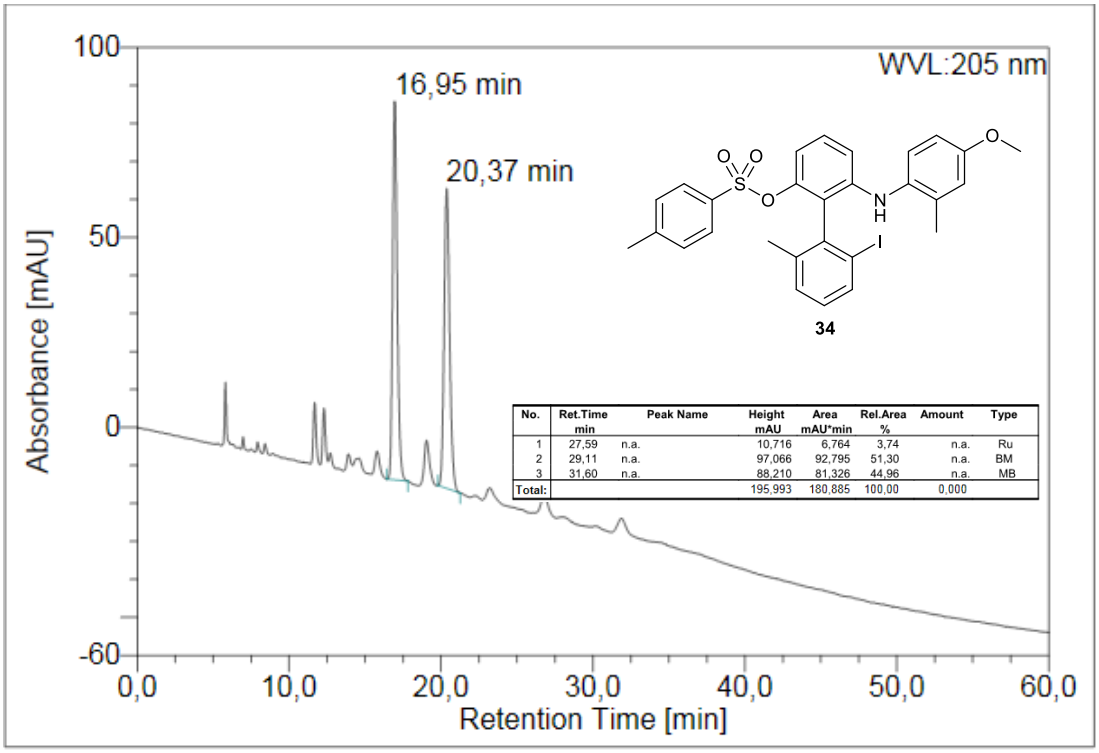
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	25,38 n.a.		217,488	177,097	50,62	n.a.	BMB
2	28,54 n.a.		183,177	172,749	49,38	n.a.	BMB*
Total:			400,665	349,846	100,00	0,000	

HPLC chromatogram of *rac*-**12**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.99/0.01 (*v*/*v*), t_R(E1): 25.38 min, t_R(E2): 28.54 min



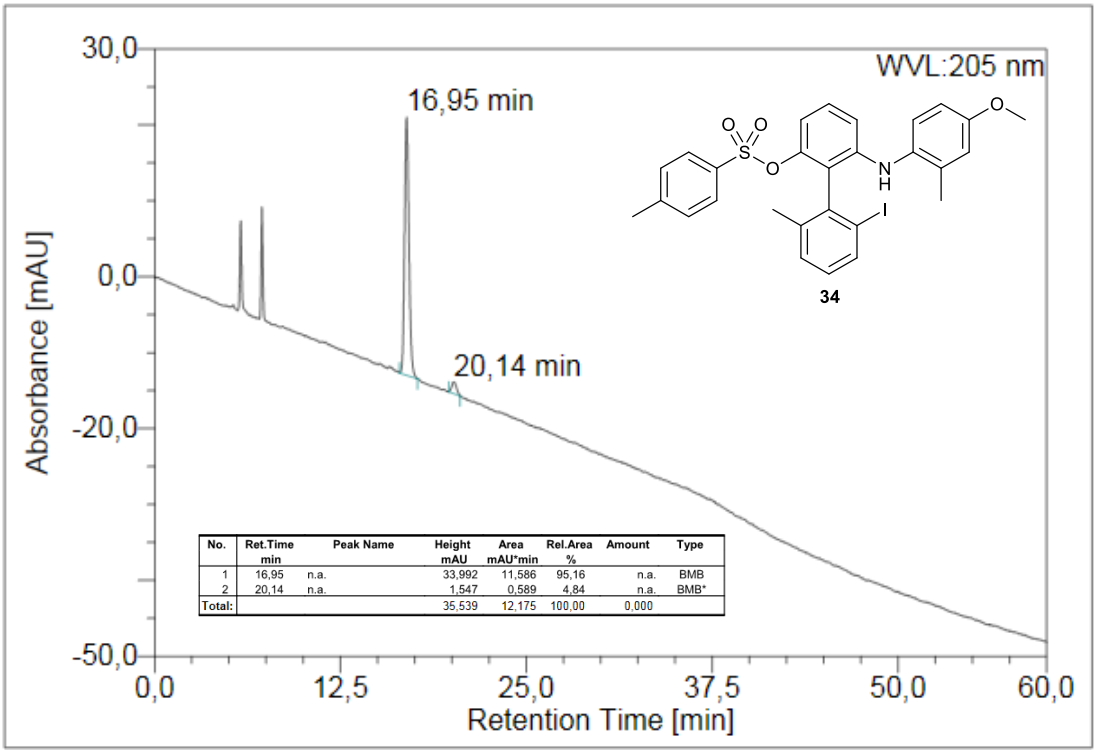
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3,31 n.a.		11,524	2,013	1,23	n.a.	BMB
2	14,57 n.a.		271,198	143,856	88,08	n.a.	BMB
3	16,48 n.a.		29,009	17,456	10,69	n.a.	BMB
Total:			311,731	163,325	100,00	0,000	

HPLC chromatogram of **12**, Chiralcel® OD-H (Daicel) 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99.99/0.01 (*v*/*v*), t_R(E1): 25.22 min, t_R(E2): 28.52 min, 77%*ee*



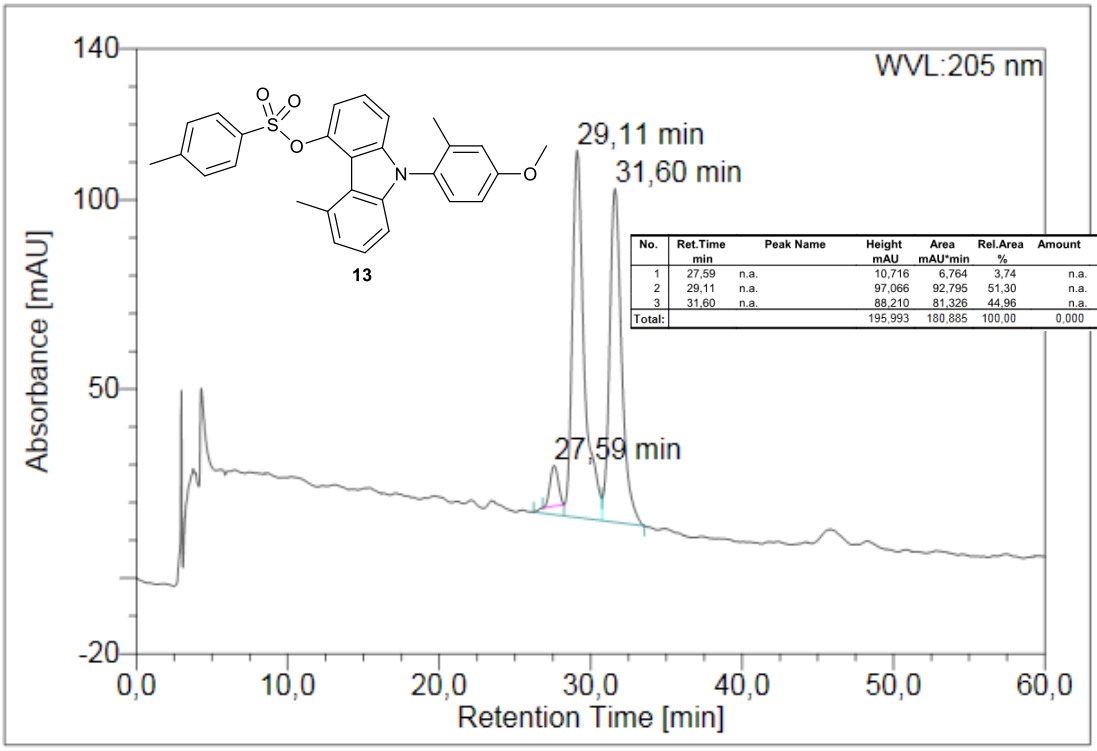
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	27,59	n.a.	10,716	6,764	3,74	n.a.	Ru
2	29,11	n.a.	97,066	92,795	51,30	n.a.	BM
3	31,60	n.a.	88,210	81,326	44,96	n.a.	MB
Total:			195,993	180,885	100,00	0,000	

HPLC chromatogram of *rac*-**34**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 90/10 (*v*/*v*), t_R(E1): 16.95 min, t_R(E2): 20.37 min



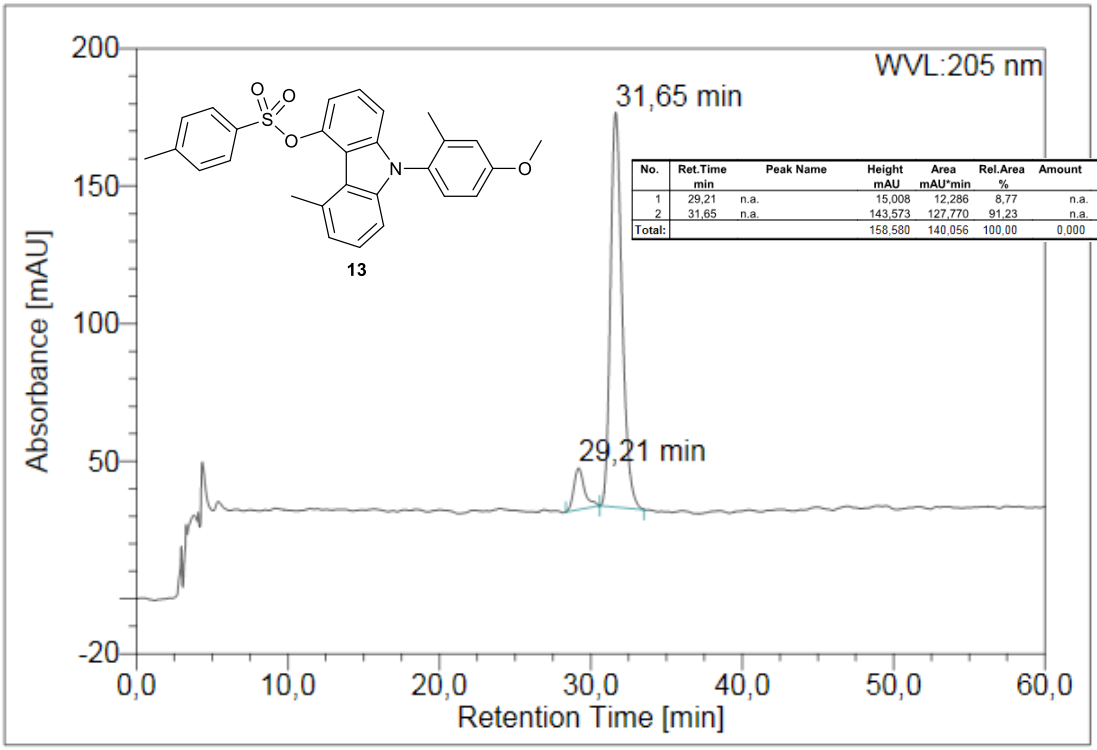
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	16,95	n.a.	33,992	11,586	95,16	n.a.	BMB
2	20,14	n.a.	1,547	0,589	4,84	n.a.	BMB*
Total:			35,539	12,175	100,00	0,000	

HPLC chromatogram of (–)-**34**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 90/10 (*v*/*v*), t_R(E1): 16.95 min, t_R(E2): 20.14 min, 90%*ee*



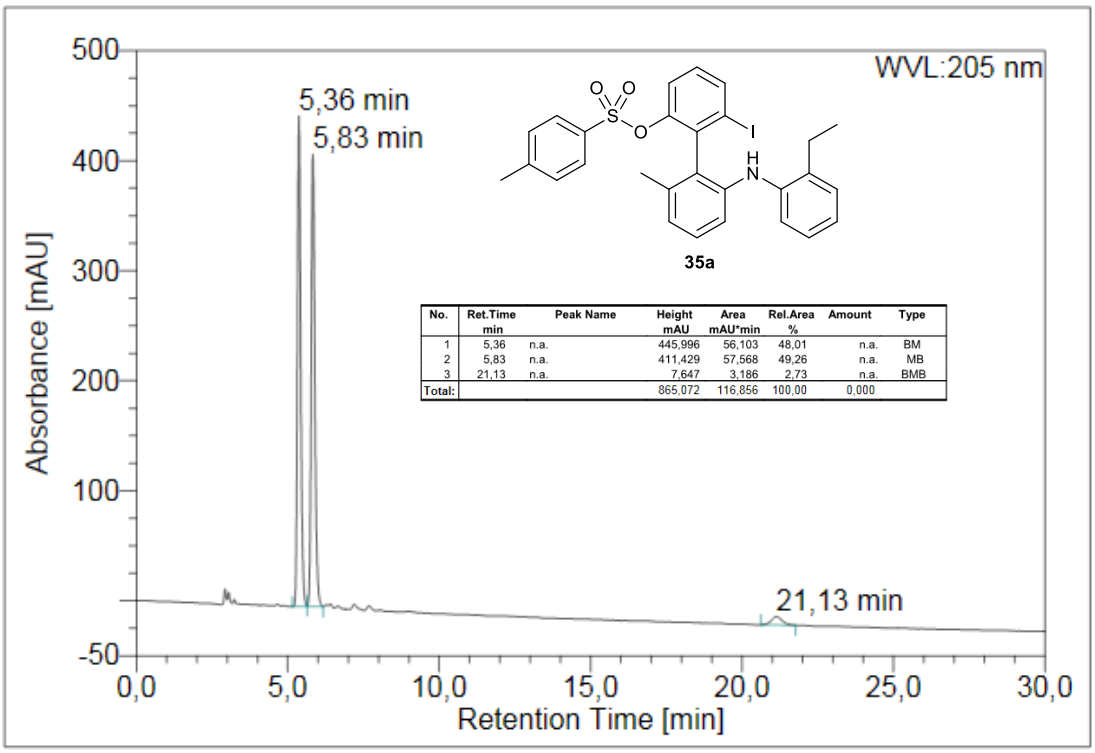
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	27,59	n.a.	10,716	6,764	3,74	n.a.	Ru
2	29,11	n.a.	97,066	92,795	51,30	n.a.	BM
3	31,60	n.a.	88,210	81,326	44,96	n.a.	MB
Total:			195,993	180,885	100,00	0,000	

HPLC chromatogram of *rac*-**13**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 15 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 29.11 min, t_R(E2): 31.60 min



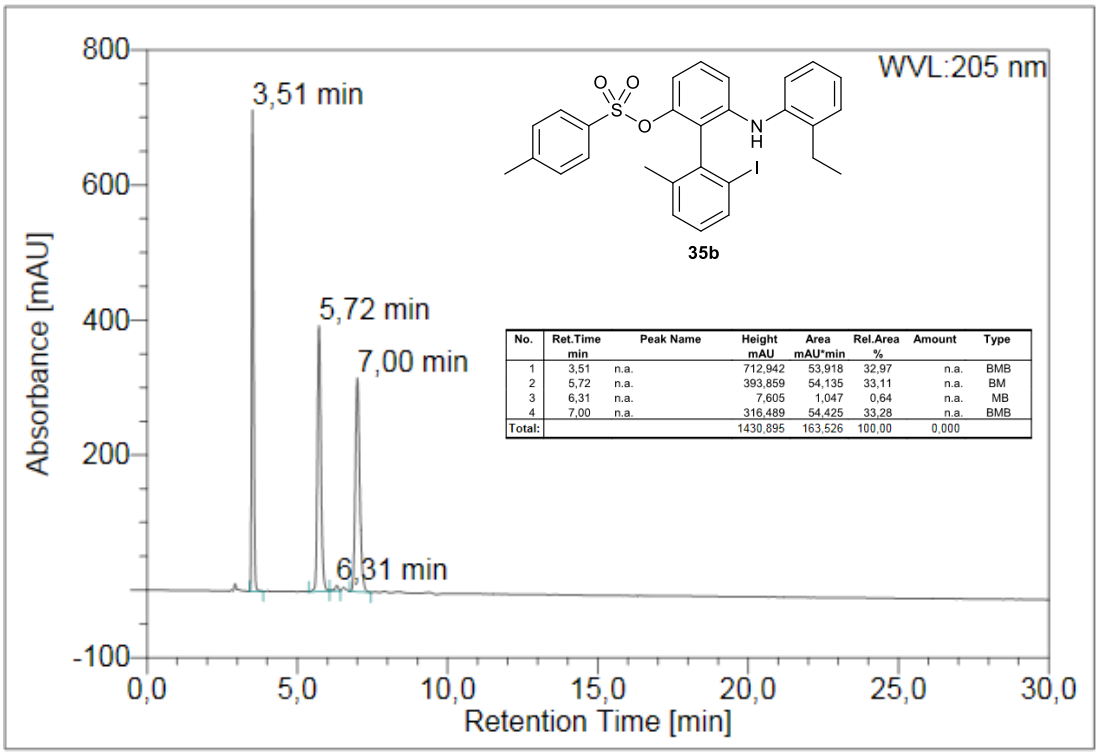
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	29,21	n.a.	15,008	12,286	8,77	n.a.	BMb*
2	31,65	n.a.	143,573	127,770	91,23	n.a.	bMB
Total:			158,580	140,056	100,00	0,000	

HPLC chromatogram of (–)-**13**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 15 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 29.21 min, t_R(E2): 31.65 min, 82% *ee*



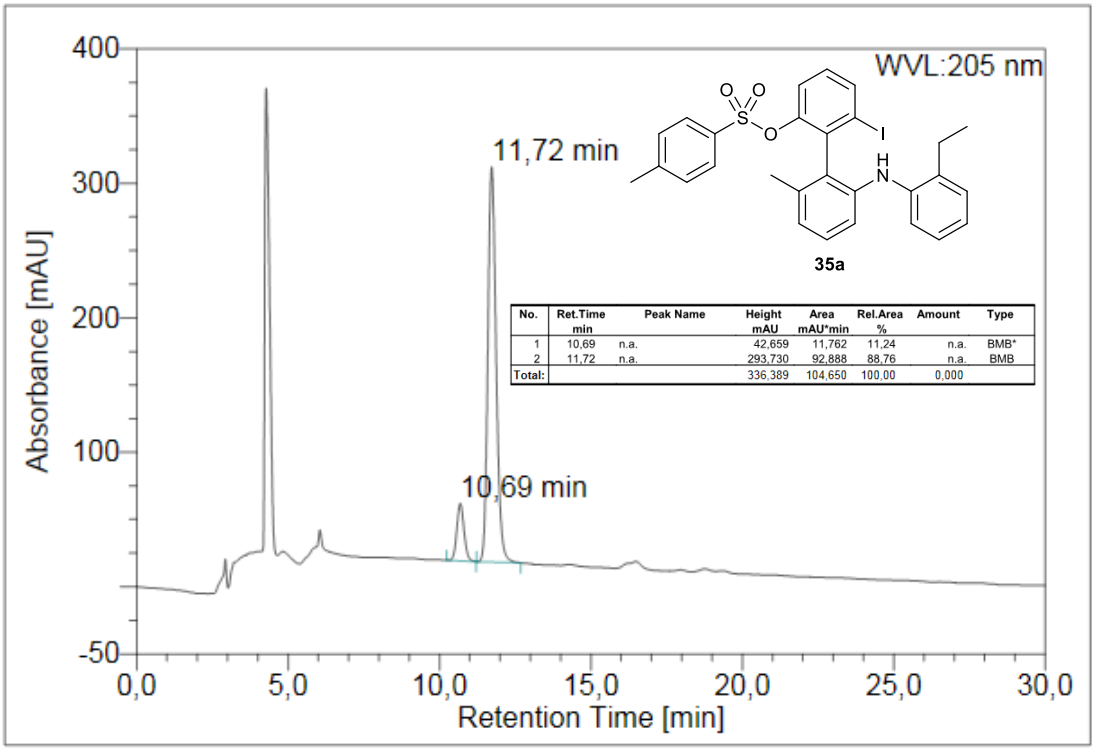
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5,36	n.a.	445,996	56,103	48,01	n.a.	BM
2	5,83	n.a.	411,429	57,568	49,26	n.a.	MB
3	21,13	n.a.	7,647	3,186	2,73	n.a.	BMB
Total:			865,072	116,856	100,00	0,000	

HPLC chromatogram of *rac*-**35a**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 95/5 (*v*/*v*), t_R(E1): 5.36 min, t_R(E2): 5.83 min



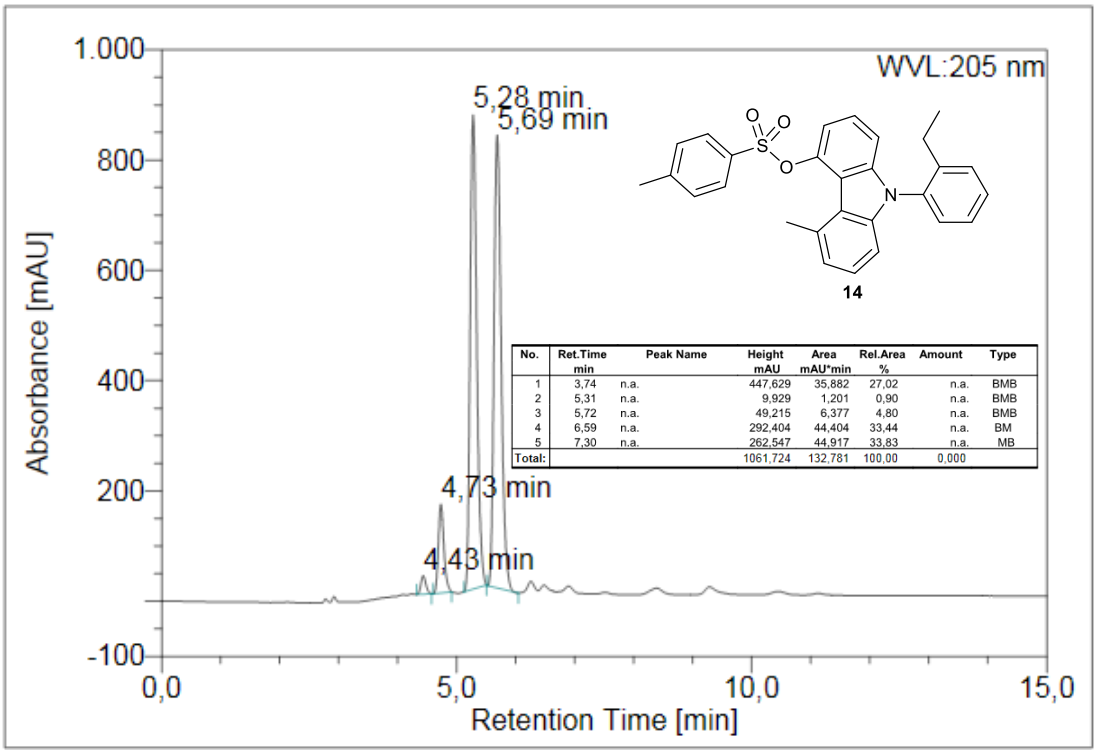
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3,51	n.a.	712,942	53,918	32,97	n.a.	BMB
2	5,72	n.a.	393,859	54,135	33,11	n.a.	BM
3	6,31	n.a.	7,605	1,047	0,64	n.a.	MB
4	7,00	n.a.	316,489	54,425	33,28	n.a.	BMB
Total:			1430,895	163,526	100,00	0,000	

HPLC chromatogram of *rac*-**35b**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 90/10 (*v*/*v*), t_R(EtOAc): 3.51 min, t_R(E1): 5.72 min, t_R(E2): 7.00 min



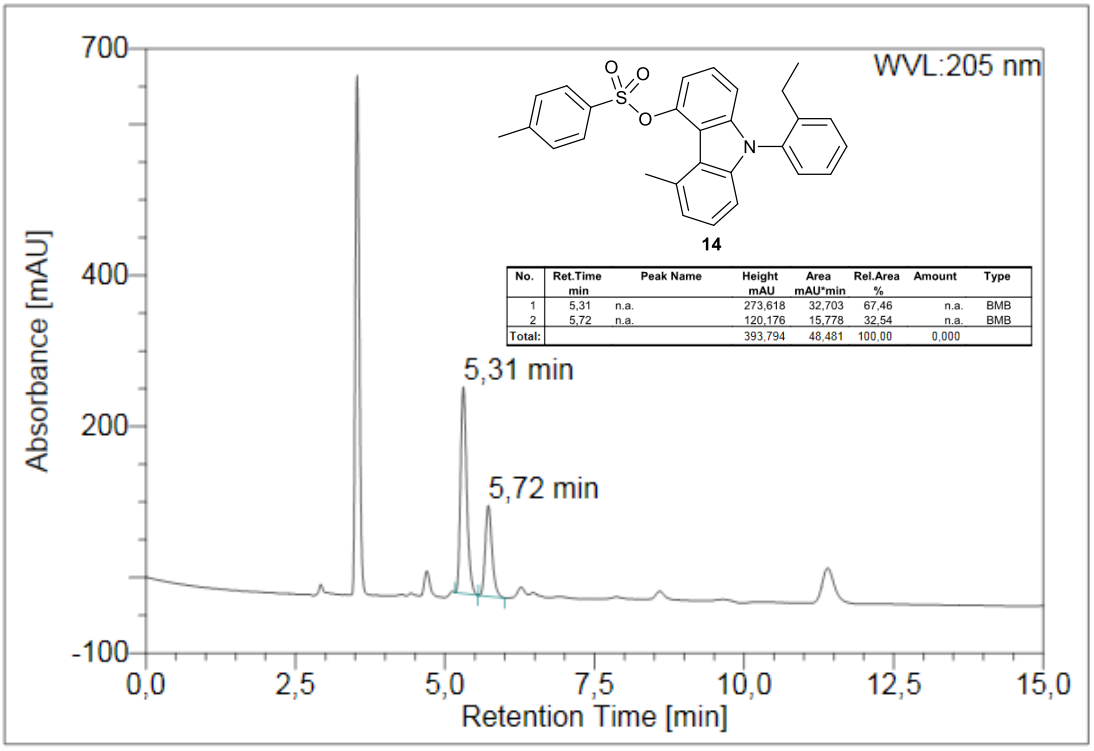
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	10,69	n.a.	42,659	11,762	11,24	n.a.	BMB*
2	11,72	n.a.	293,730	92,888	88,76	n.a.	BMB
Total:			336,389	104,650	100,00	0,000	

HPLC chromatogram of **35a**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 99/1 (*v*/*v*), t_R(E1): 10.69 min, t_R(E2): 11.72 min, 78% *ee*



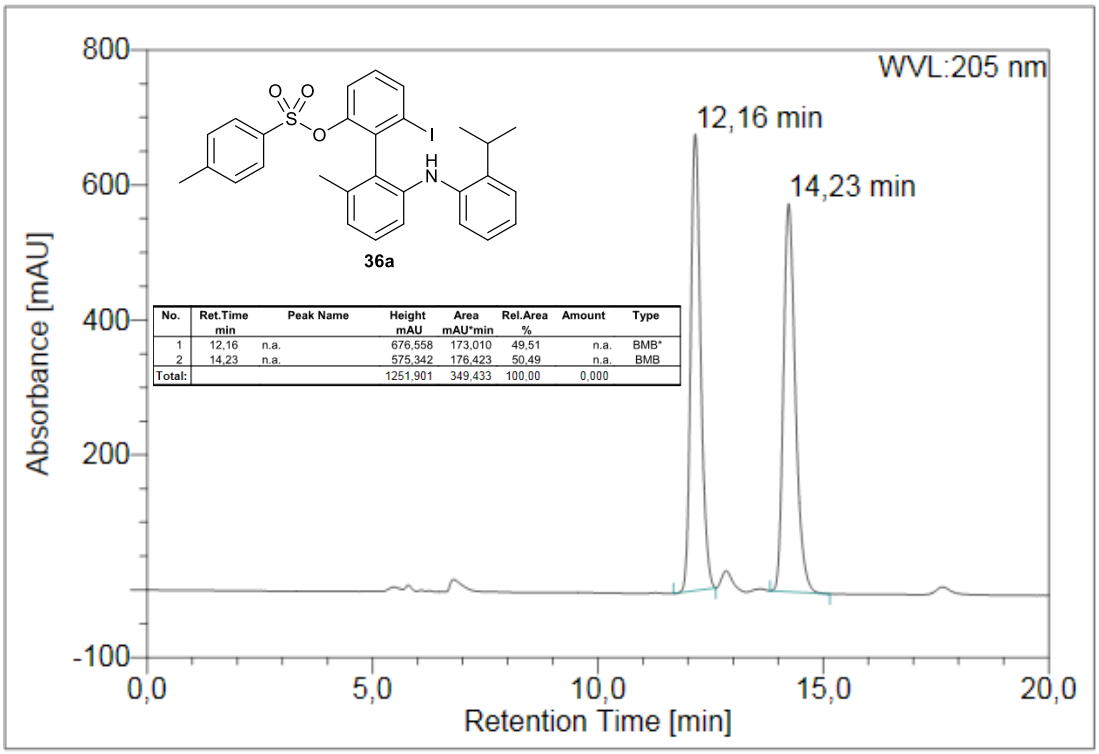
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	3,74	n.a.	447,629	35,882	27,02	n.a.	BMB
2	5,31	n.a.	9,929	1,201	0,90	n.a.	BMB
3	5,72	n.a.	49,215	6,377	4,80	n.a.	BMB
4	6,59	n.a.	292,404	44,404	33,44	n.a.	BM
5	7,30	n.a.	262,547	44,917	33,83	n.a.	MB
Total:			1061,724	132,781	100,00	0,000	

HPLC chromatogram of *rac*-**14**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 90/10 (*v*/*v*), t_R(E1): 5.28 min, t_R(E2): 5.69 min



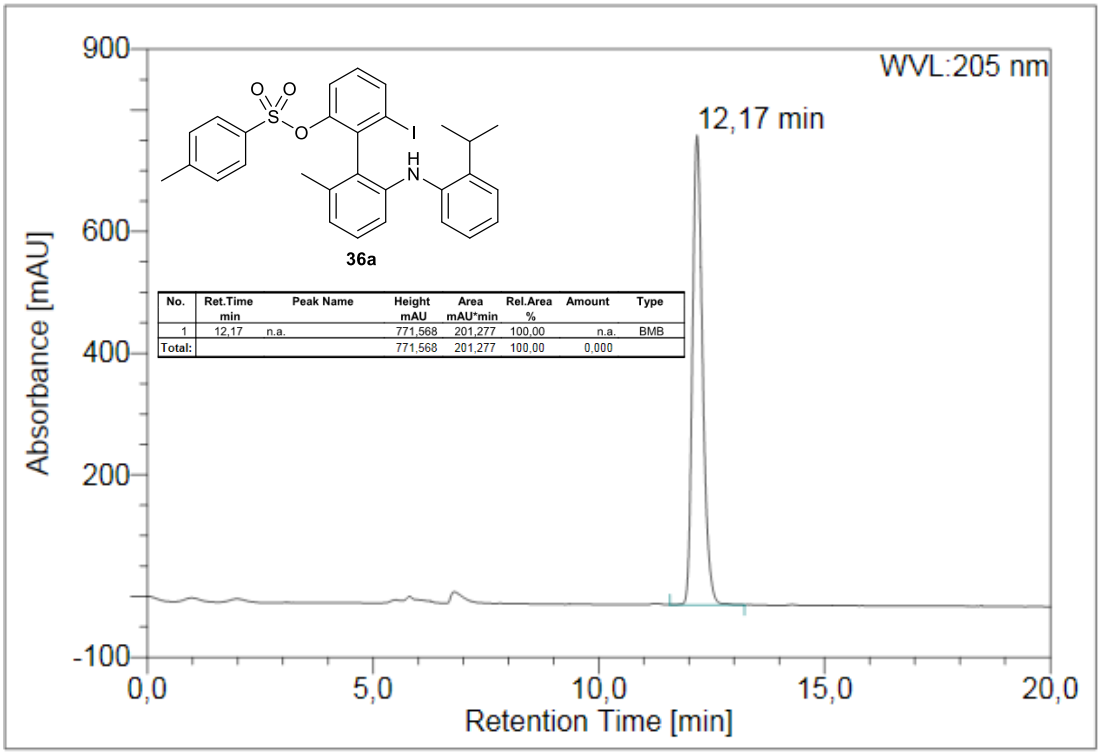
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	5,31	n.a.	273,618	32,703	67,46	n.a.	BMB
2	5,72	n.a.	120,176	15,778	32,54	n.a.	BMB
Total:			393,794	48,481	100,00	0,000	

HPLC chromatogram of **14**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 90/10 (*v*/*v*), t_R(EtOAc): 3.53 min, t_R(E1): 5.31 min, t_R(E2): 5.72 min, 35% *ee*



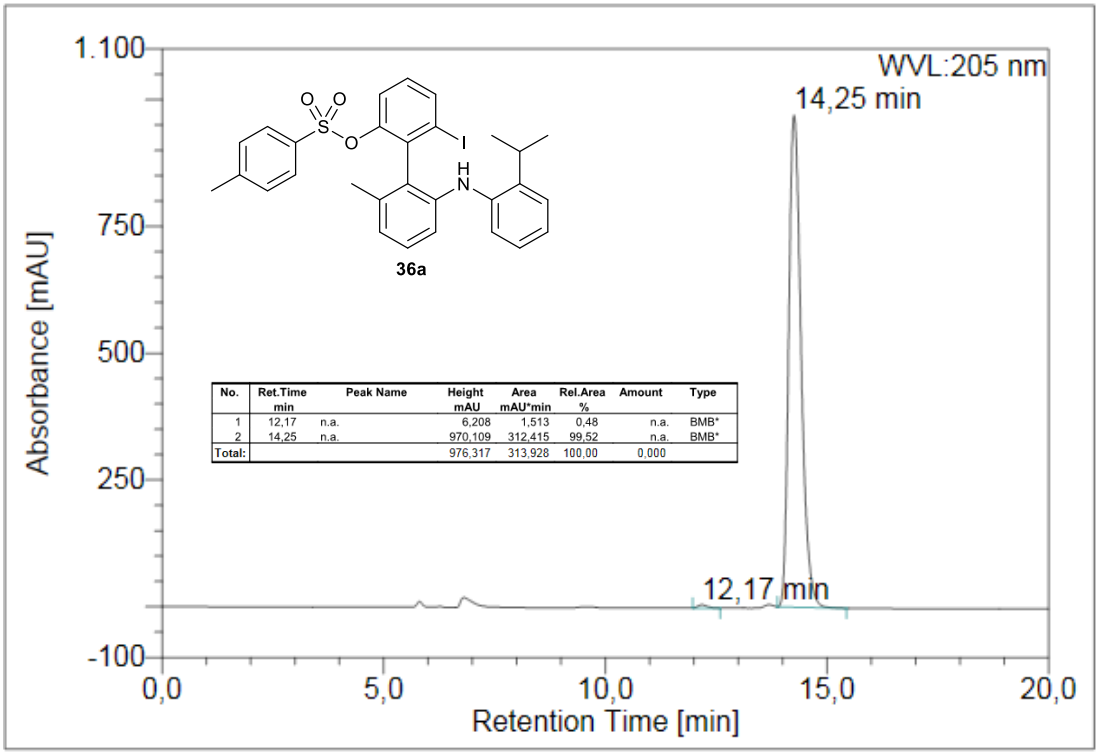
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12,16	n.a.	676,558	173,010	49,51	n.a.	BMB*
2	14,23	n.a.	575,342	176,423	50,49	n.a.	BMB
Total:			1251,901	349,433	100,00	0,000	

HPLC chromatogram of *rac*-**36a**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 98/2 (*v*/*v*), t_R(E1): 12.16 min, t_R(E2): 14.23 min



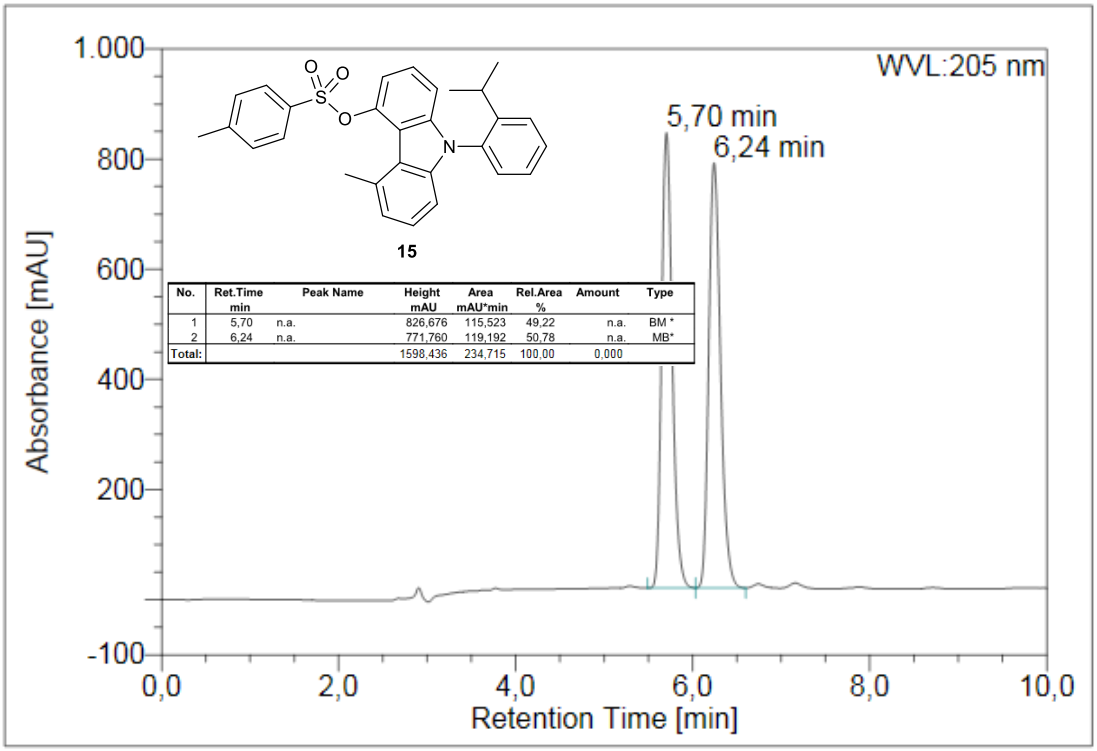
No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12,17	n.a.	771,568	201,277	100,00	n.a.	BMB
Total:			771,568	201,277	100,00	0,000	

HPLC chromatogram of (–)-**36a**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 98/2 (*v*/*v*), t_R(E1): 12.17 min, >99% *ee*

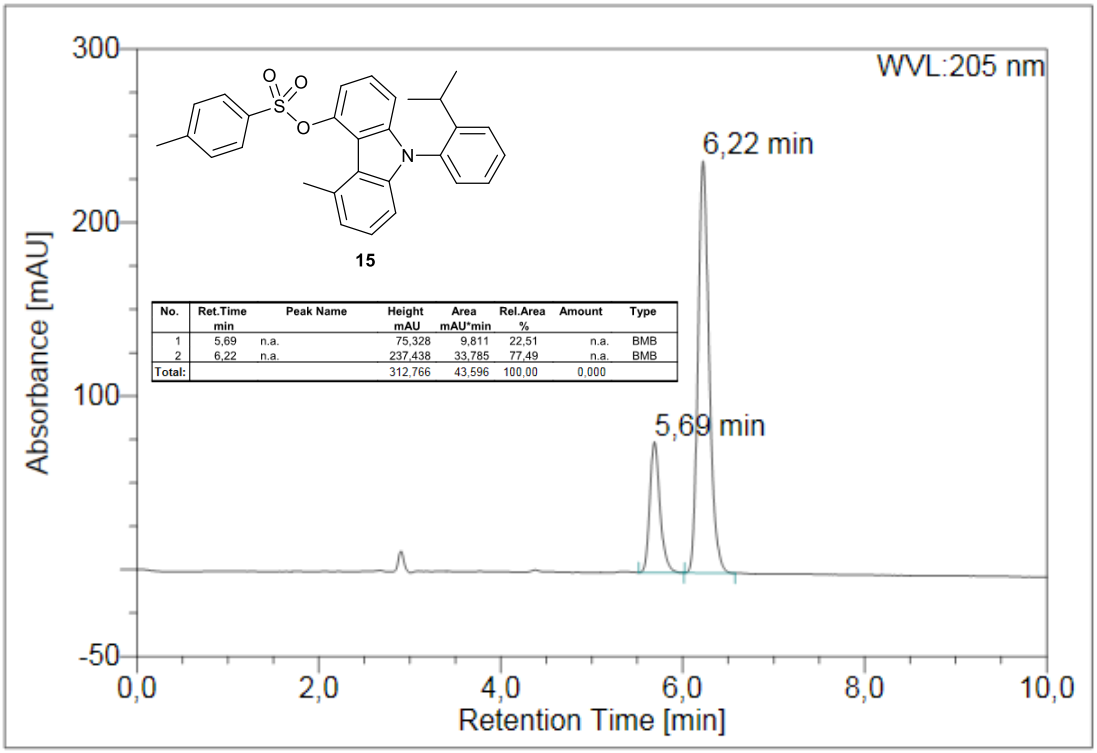


No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	12,17	n.a.	6,208	1,513	0,48	n.a.	BMB*
2	14,25	n.a.	970,109	312,415	99,52	n.a.	BMB*
Total:			976,317	313,928	100,00	0,000	

HPLC chromatogram of (+)-**36a**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 0.5 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 98/2 (*v*/*v*), t_R(E1): 12.17 min, t_R(E2): 14.25 min, 99% *ee*



HPLC chromatogram of *rac*-**15**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 95/5 (*v*/*v*), t_R(E1): 5.70 min, t_R(E2): 6.24 min



HPLC chromatogram of (–)-**15**, Lux® Amylose-1 (Phenomenex), 250 × 4.6 mm, 25 °C, 1 ml/min, 205 nm, *n*-heptane/*i*-PrOH: 95/5 (*v*/*v*), t_R(E1): 5.69 min, t_R(E2): 6.22 min 56% *ee*