Direct Access to Alkylideneoxindoles *via* Axially-Enantioselective Knoevenagel Condensation.

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Contents

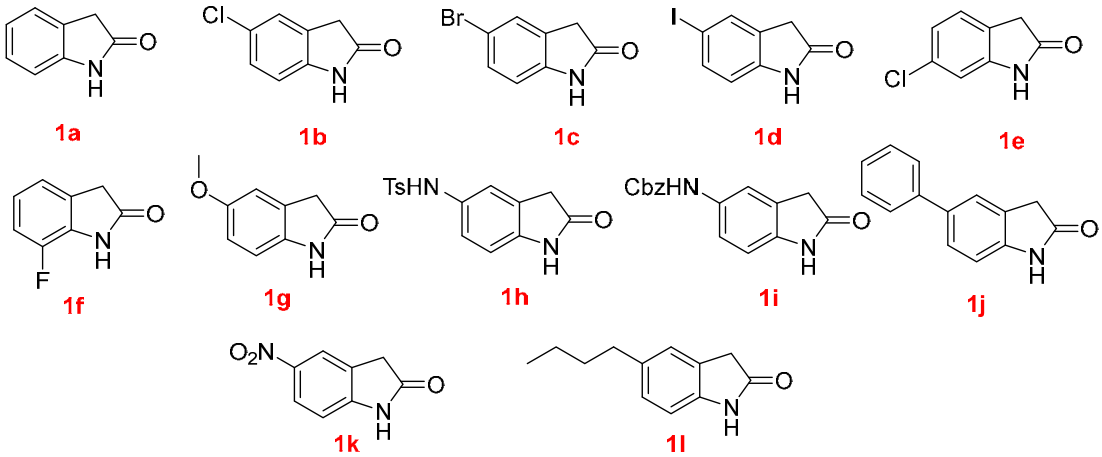
General

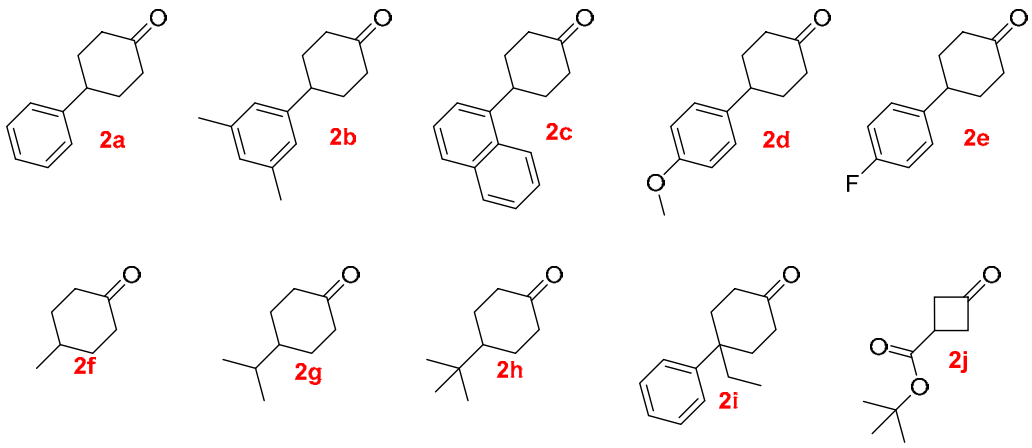
All the NMR spectra were recorded on Inova 300 MHz, Gemini 400 MHz or Mercury 600 MHz Varian spectrometers for ^{1}H, 75 MHz, 100 MHz and 150 MHz for ^{13}C and 282 MHz, 376 MHz, 564 MHz for ^{19}F respectively. The chemical shifts (δ) for ^{1}H, ^{19}F and ^{13}C are given in ppm relative to internal standard TMS (0.0 ppm) or residual signals of $CHCl_3$ (7.26 ppm) or DMSO (2.48 ppm). Coupling constants are given in Hz. The following abbreviations are used to indicate the multiplicity: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; bs, broad signal. Purification of reaction products was carried out by flash chromatography (FC) on silica gel (230-400 mesh). Organic solutions were concentrated under reduced pressure on a Büchi rotary evaporator. High Resolution Mass spectra were obtained from the CIGS facilities of the University of Modena and Reggio Emilia on a G6520AA Accurate-Mass Q-TOF LC/MS instrument. Chiral HPLC analysis was performed on an Agilent 1100-series instrumentation. HPLC traces for all compounds were compared to *quasi* racemic samples prepared by mixing the two product antipodes obtained performing the reactions with catalyst **VII** and the *pseudo*-enantiomer **VIII** separately. Since the crude reaction mixture was in all cases enough clean to allow the direct hplc analysis, the spectra reported in the dedicate section are relative to the crude mixture. Optical rotations have not been determined due to a partial instability of the products if stored for long period and exposed to light even for few hours. All reactions were carried out without any precaution to exclude moisture and oxygen. Chiral catalyst **I** and **V** are commercially available. Catalyst **II**,[1] **III**,[1] **IV**,[1] **VI**,[2] **VII**,[3] **VIII**,[3] **IX**,[3] **X**,[4] **XI**[3] were prepared following literature procedures. Oxindoles **1a**, **1b**, **1c**, **1e**, **1f** and **1i** were commercially available. Oxindole **1d**,[5] **1h**,[6] **1i**,[7] **1j**[8] were prepared following the literature procedure and their NMR spectra were consistent with those previously reported. Cyclohexanones **2a**, **2f**, **2g**, **2h** and **2j** were commercially available.

[1] Kim H.; Nguyen, Y.; Pai-Hui C.; Leonid Chagal, Y.;. Lough, A. J.; Moon Kim, B.; Chin, J. *J. Am. Chem. Soc.*, **2008**, *130*, 12184.
[2] Badiola, E.; Fiser, B.; Gomez-Bengoa, E.; Mielgo, A.; Olaizola, I.; Urruzuno, I.; García, J. M.; Odriozola, J. M.; Razkin, J.; Mikel Oiarbide, M.; Palomo, C. *J. Am. Chem. Soc.*, **2014**, *136*, 17869.
[3] (a) Cassani, C.; Martín-Rapún, R.; Arceo, E.; Bravo, F.; Melchiorre, P. *Nature Protocols* **2013,** *8*, 325.
[4] Lee, A.; Michrowska, A.; Mosse-Sulzer, S.; List, B. *Angew. Chem. Int. Ed.*, **2011**, *50*, 1707.
[5] (a) A. Alanine, B. Buettelmann, M. P. H. Neidhart, G. Jaeschke, E. Pinard, R. Wyler US2001/47031, **2001**, A1. (b) M. Kuchara, M. C. Oliveira, L. G. I. Santos, T. Kniess *Bioorg. Med. Chem. Lett.* **2012**, *22*, 2850.
[6] S. Raposelli, C. Martini, V. Calderone, G. Puricelli (International Society for drug development) WO2016/55454, **2016**, A1.
[7] T. P. Cho, H. G. Davis; L. Xiaoyuan US2002/52369, **2002**, A1.
[8] S. Göring, J.-M. Taymans, V. Baekelandt, B. Schmidt *Bioorg. Med. Chem. Lett.* **2014**, *24*, 4630.

Ketones **2b**, **2c**, **2d**, **2e** and **2i** have been prepared following the literature procedures[9] and their NMR spectra were consistent with those previously reported.

Oxindoles and Ketones use for the *a*EKC

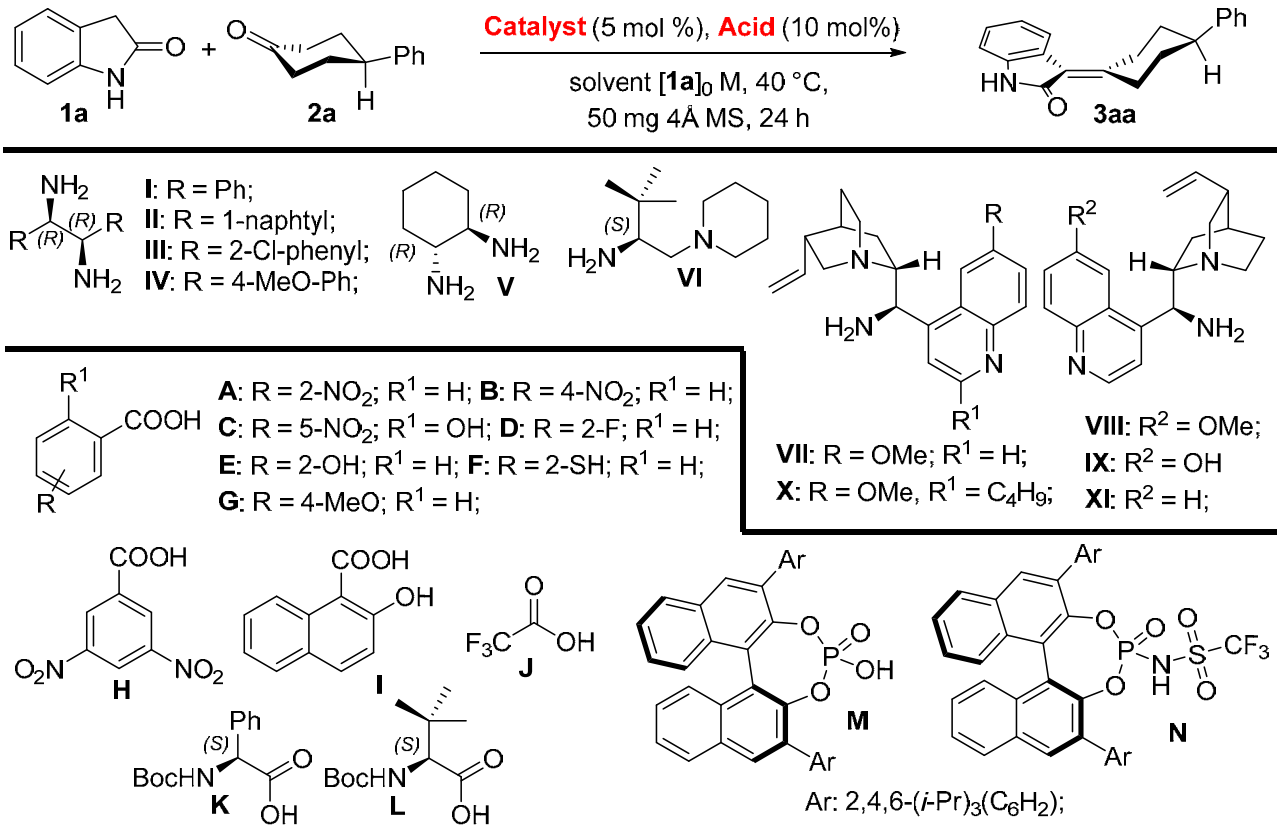




[9] (a) S. Müller, M. J. Webber, B. List, *J. Am. Chem. Soc.* **2011**, *133*, 18534. (b) A. R. Ekkati, V. Mandiyan, K. P. Ravindranathan, J. H. Bae, J. Schlessinger, W. L. Jorgensen, *Tetrahedron Lett.*, **2011**, *52*, 2228. (c) Y. Naganawa, M. Kawagishi, J. I. Ito, H. Nishiyama *Angew. Chem. Int. Ed.*, **2016**, *55*, 6873.

Screening of the reaction conditions

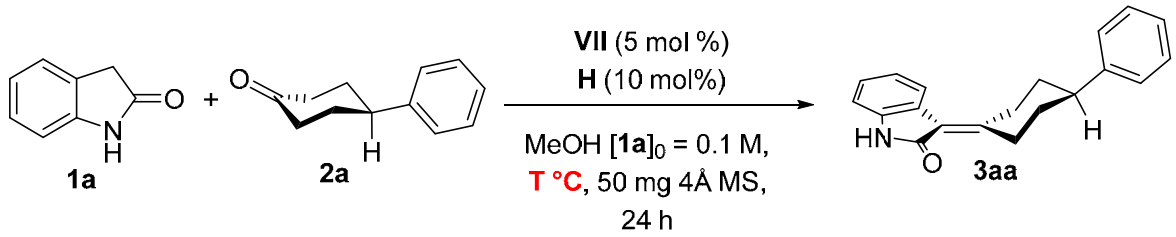
Table S1: Screening of organocatalyst[a]



Entry	Catalyst	Acid	Solvent	Yield (%)[b]	E.r.[c]
1	I	H	MeOH	12	34:66
2	II	H	Toluene	17	18:82
3	III	H	Toluene	46	25:75
4	IV	H	Toluene	13	19.5:80.5
5	V	H	Toluene	28	37:63
6[d]	VI	H	MeOH	----	-----
7	VII	H	MeOH	55	14:86
8	VIII	H	MeOH	52	85:15
9[d]	IX	H	MeOH	----	-----
10	X	H	MeOH	49	14:86
11	XI	H	MeOH	45	87:13
12[e]	VII	H	MeOH	8	41:59

[a]Reactions were performed using 0.2 mmol of **1a** and 0.2 mmol of **2a**. [b]Isolated yield. [c]Determined by HPLC using chiral stationary phase [d]No product was obtained. [e]Reaction without Molecular Sieves.

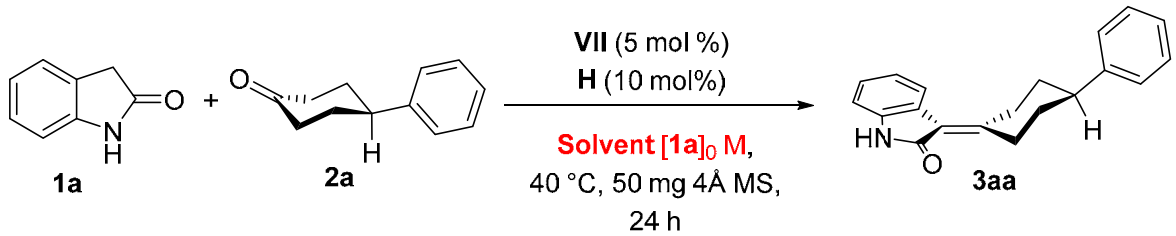
Table S2: Screening of temperature[a]



Entry	Temperature (°C)	Yield (%)[b]	E.r.[c]
1	25	24	15:85
2	40	55	14:86

[a]Reactions were performed using 0.2 mmol of **1a** and 0.2 mmol of **2a**. [b]Isolated yield. [c]Determined by HPLC using chiral stationary phase

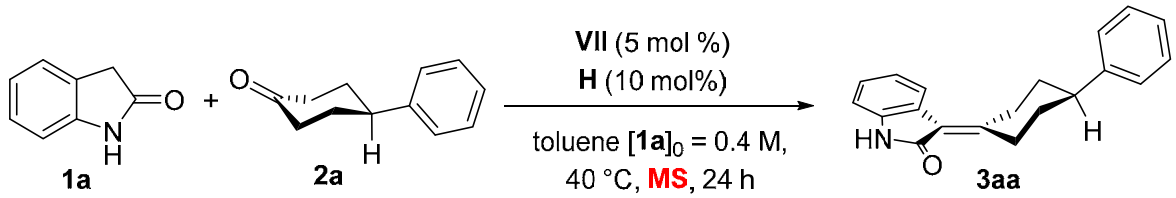
Table S3: Screening of solvent[a]



Entry	Solvent	$[1a]_0$ M	Yield (%)[b]	E.r.[c]
1	MeOH	0.1	55	14:86
2	Toluene	0.1	63	14:86
3	*i*PrOH	0.1	18	15:85
4	Tetrahydrofuran	0.1	49	26:74
5	Chlorobenzene	0.1	50	19:81
6	Dichloromethane	0.1	22	22:78
7	Dimethylsulfoxide	0.1	18	20:80
8	Toluene	0.4	90	13:87
9	Toluene	0.7	62	14:86
10	Toluene	1.0	64	13:87

[a]Reactions were performed using 0.2 mmol of **1a** and 0.2 mmol of **2a**. [b]Isolated yield. [c]Determined by HPLC using chiral stationary phase.

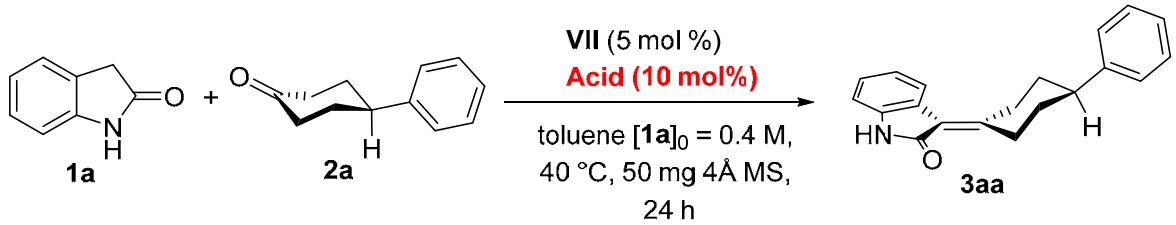
Table S4: Screening of molecular sieves[a]



Entry	Molecular Sieves (mg)	Yield (%)[b]	Ee (%)[c]
1	4 Å (50)	90	13:87
2[d]	4 Å (50)	90	14:86
3	5 Å (50)	n.d.	15:85
4	3 Å (50)	n.d.	14:86

[a]Reactions were performed using 0.2 mmol of **1a** and 0.2 mmol of **2a**. [b]Isolated yield. [c]Determined by HPLC using chiral stationary phase. [d]Powdered MS were used.

Table S5: Screening of acids[a]



Entry	Acid (mol%)	Yield (%)[b]	E.r.[c]
1	A	70	13.5:86.5
2	B	45	12:88
3	C	62	20:80
4	D	n.d.	19:81
5	E	60	14:86
6	F	n.d.	19:81
7	G	43	15:85
8	H	90	13:87
9	I	n.d.	22:78
10[d]	J	-----	----
11	K	12	20:80
12	L	28	19:81
13	M	<10	20:80
14	N	<10	20:80

[a]Reactions were performed using 0.2 mmol of **1a** and 0.2 mmol of **2a**. [b]Isolated yield. [c]Determined by HPLC using chiral stationary phase [d]No product was obtained.

Determination of the absolute configuration

Despite several efforts, crystals suitable for X-ray diffraction (XRD) analysis could not be obtained. Therefore, absolute configuration was assigned by comparison of the experimental electronic circular dichroism (ECD) with that calculated by time-dependent density functional theory (TD-DFT). Quantum-mechanical (QM) calculations of chiroptical properties has become easily accessible and a widespread tool for assigning absolute configurations of several classes of molecules.[10]

Conformational searching

The (a*R*) configuration of the product was arbitrarily chosen and a molecular mechanics (MM) conformational search was run using the Merck molecular force-field (MMFF) as implemented in the SCAN application of the TINKER molecular modeling package.[11] The search was run starting from both structures with the phenyl group in the axial and in the equatorial disposition of the cyclohexylidene ring. The search yielded three different conformations within a range of 10 kcal/mol from the lowest one. These three structures were then quickly optimized using DFT[12] at the B3LYP/3-21G level of theory eliminating duplicates. This first round of optimization yielded only two conformations corresponding to different geometries, one with the phenyl group in the equatorial disposition and the other with the phenyl group in the axial disposition.

These two conformations were further optimized both at the B3LYP/6-311+G(2d,p) and at M06-2X/6-311+G(2d,p) level of theory, without noting any significant difference between the structures computed with the B3LYP and the M06-2X functionals. Therefore, the B3LYP geometries were used in the following steps.

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[10] For reviews and examples, see: (a) G. Pescitelli, T. Bruhn *Chirality* **2016**, *28*, 466; (b) C. Adamo, D. Jacquemin *Chem. Soc. Rev.,* **2013**, *42*, 845; (c) A. E. Nugroho, H. Morita *J Nat Med* **2013**; *68*, 1.

[11] TINKER 8: A Modular Software Package for Molecular Design and Simulation. Joshua A. Rackers, Marie L. Laury, Chao Lu, Zhi Wang, Louis Lagardère, Jean-Philip Piquemal, Pengyu Ren, Jay W. Ponder, **2018**.

[12] All QM computations were performed using Gaussian 16, Revision A.03, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

Finally, the gas-phase geometries were reoptimized at the same B3LYP/6-311+G(2d,p) level, this time including the solvent effect (polarizable continuum model, PCM) both in *n*-hexane and in 2-propanol. Again, no significant difference was noted between the geometry obtained for *n*-hexane and that obtained for 2-propanol and therefore the geometry optimized at the PCM(*n*-hexane)/-B3LYP/ 6-311+G(2d,p) was used for the following steps. All geometries obtained were verified to be minima by running a frequency calculation at the same level of theory that showed the absence of any imaginary frequency. The two final conformations (Fig. 1) were found to be separated by 3.42 kcal/mol.[13] Thus the minor axial conformer contributes less than 0.5% to the Boltzmann distribution and the following TD-DFT computations were run only for the major equatorial conformer.

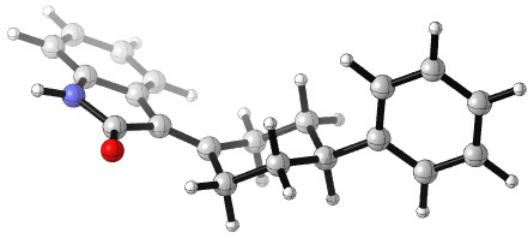
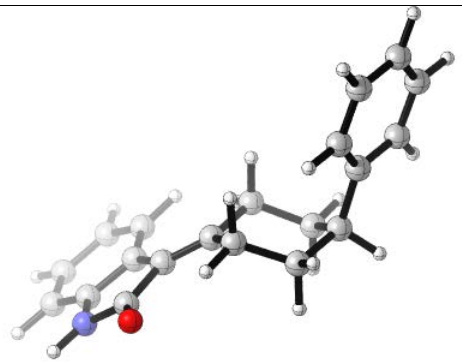
	
equatorial (E = 0.00 kcal/mol)	axial (E = 3.42 kcal/mol)

Fig. S1.[14] Geometries of the equatorial and axial conformations of the (a*R*)-enantiomer calculated with the B3LYP/6-311+G(2d,p) model chemistry.

Torsional twist at the C=C double bond

The computed minimum (Fig. 1) has a slight torsional twist at the C=C double bond: the dihedral angle θ (C1-C2-C3-C4) is equal to +7.4° (Fig. 2). This forces the carbonyl oxygen in a *sin* disposition with respect to the phenyl group. Particular care was devoted to find if also the *anti* conformation is populated. In fact, this conformation is diastereomeric to the *sin* (Fig. 2) and might contribute differently to the ECD spectrum. Indeed, preliminary calculations showed that the geometry of the compound X where the θ angle was arbitrarily fixed at -7.4° (*anti* conformation) has very different chiroptical properties with respect to those computed for the *sin* conformer. For example, they show very different computed optical rotations.

[13] This is Gaussian "Electronic Energy (EE)". Similar values were obtained considering: zero-point energy correction (3.63 kcal/mol); thermal correction to energy (3.53 kcal/mol); thermal correction to enthalpy (3.52 kcal/mol) or thermal correction to free energy (3.89 kcal/mol)

[14] CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

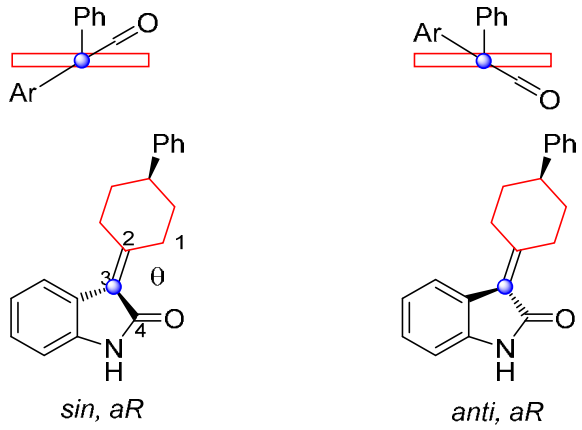


Fig. S2. Possible diastereomeric conformations of **3aa** arising from a torsional twist of the C=C double bond; *sin* and *anti* refer to the disposition of the oxygen atom with respect of that of the phenyl group.

Then, starting from the computed minimum (Fig. S1), a relaxed potential energy surface (PES) scan was performed by varying the dihedral angle θ of the C=C double bond from 21° (*sin*) to -18° (*anti*) with a 3° step. The energy profile that was obtained is showed in Fig. S3.

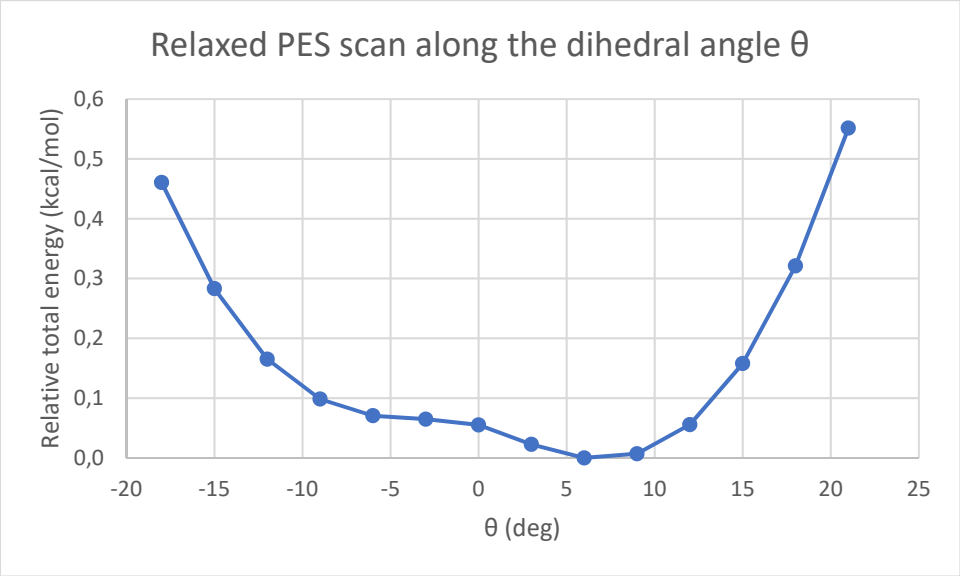


Fig. S3. Result of the relaxed PES scan along the dihedral angle θ.

The profile in figure S3, does not allow to safely rule out that a very shallow energy well might exist at a θ value around -6° and hence that a very low barrier *anti* conformation might be populated. This conformation would be about 0.8 kcal/mol above the computed minimum with a Boltzmann distribution of about 20% at 298 K. In the attempt to find if this *anti* conformation exists, the geometry with θ value of -12° from the previous PES scan was used as the starting geometry for a careful minimum search. Any constrain was removed and DFT calculations at the B3LYP/6-

311+G(2d,p) with a very tight convergence criteria were performed. The calculation was repeated several times also using maximum step sizes of ½ and 1/3 of the default one. No *anti* conformation was found from these calculations as they always yielded the already known *sin* conformation which therefore was the only one considered in the following ECD simulations.

Absolute configuration.

Absolute configuration was assigned by comparison of experimental electronic circular dichroism (ECD) spectrum to that calculated by TD-DFT methods. The experimental ECD spectrum of a solution of compound **3aa** in a 60:40 mixture of HPLC-grade hexane/2-propanol (about $1 \cdot 10^{-4}$ M) was acquired with a cell path of 0.2 cm in the 190-400 nm region by the sum of 16 scans at 50 nm/min scan rate (Fig. S4). The spectrum shows a broad positive band at 258 nm and two negative bands between 218 and 204 nm.

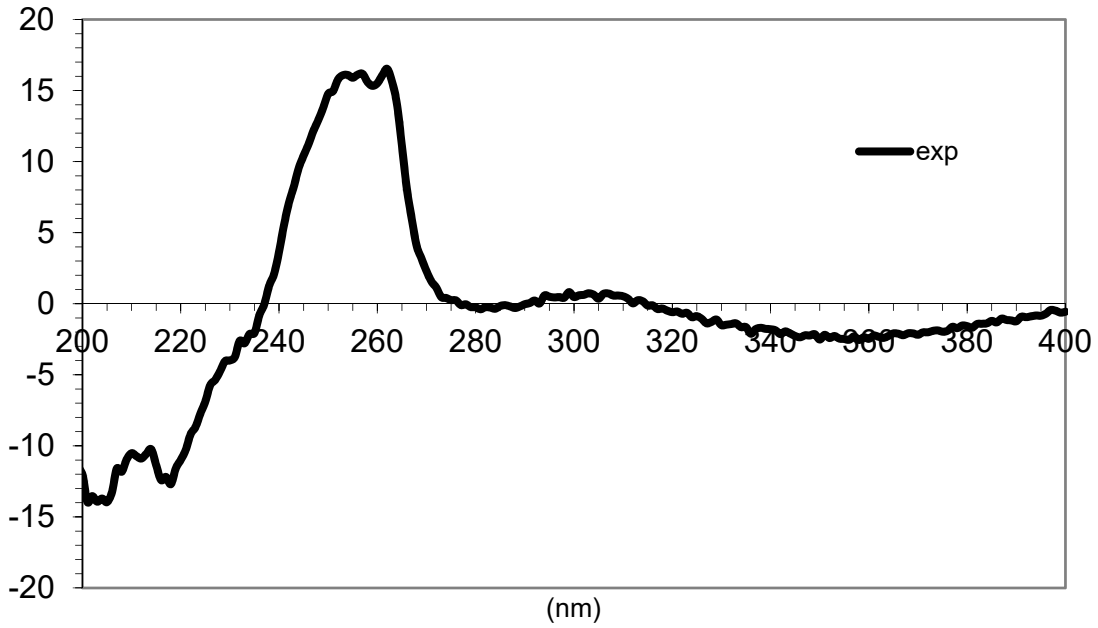


Fig. S4. Experimental ECD spectrum of compound **3aa**.

The TD-DFT simulations of the ECD spectrum of compound **3aa** were performed using the geometry of the single equatorial conformation which was found to be essentially the unique conformation populated at room temperature. For data redundancy, calculations were performed with the hybrid functionals BH&HLYP[15] and M06-2X,[16] with ωB97XD that includes empirical dispersion,[17] and with

[15] In Gaussian 09 the BH&HLYP functional has the form: $0.5*E_X^{HF} + 0.5*E_X^{LSDA} + 0.5*\Delta E_X^{Becke88} + E_C^{LYP}$

[16] Y. Zhao and D.G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.

[17] J-D. Chai and M. Head-Gordon, *Phys. Chem. Chem. Phys.*, **2008**, *10*, 6615-6620.

CAM-B3LYP[18] that includes long range correction (Fig. S5). The calculations employed the 6-311++G(2d,p) basis set, that usually yields good performances at a reasonable computational cost.[19]

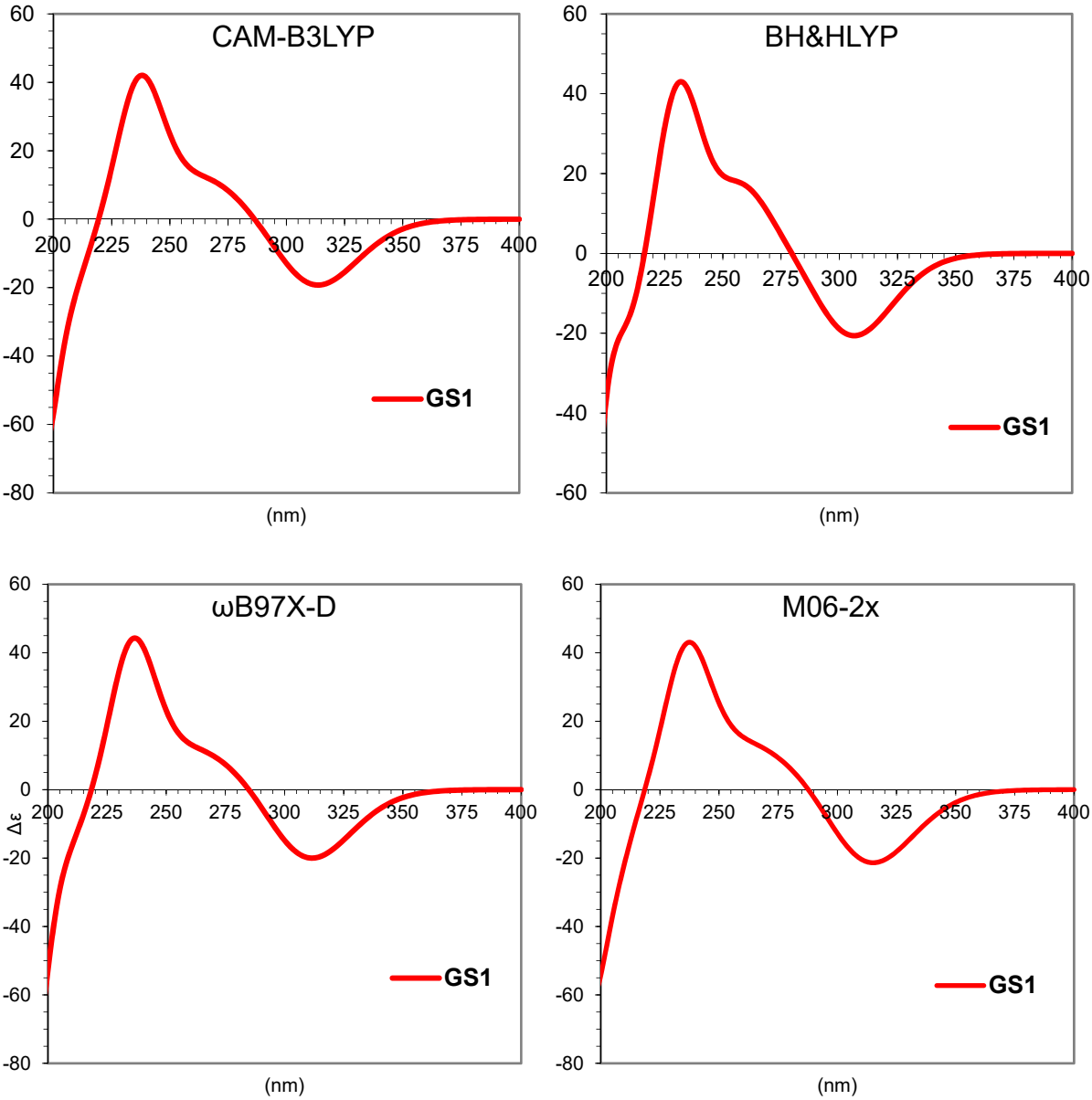


Fig. S5. TD-DFT simulated spectra calculated for of **3aa** assuming the a*R* absolute configuration and using CAM-B3LYP, BH&HLYP, M06-2X, ωB97XD and the 6-311++G(2d,p) basis set. For each conformation, the first 50 excited states were calculated, and the spectrum was obtained using a 0.25 eV line half-width at half height.

[18] T. Yanai, D. Tewand, and N. Handy, *Chem. Phys. Lett.* **2004**, *393*, 51-57.

[19] a) M. Meazza, M. E. Light, A. Mazzanti and R. Rios. *Chem. Sci.* **2016**, *7*, 984; b) P. Gunasekaran, S. Perumal, J. Carlos Menéndez, M. Mancinelli, S. Ranieri, A. Mazzanti, *J. Org. Chem.* **2014**, *79*, 11039–11050. c) L. Caruana, M. Fochi, M. Comes Franchini, S. Ranieri, A. Mazzanti, L. Bernardi, *Chem. Commun.* **2014**, *50*, 445-447. d) M. Ambrogi, A. Ciogli, M. Mancinelli, S. Ranieri, A. Mazzanti, *J. Org. Chem.* **2013**, *78*, 3709-3719. e) L. Caruana, M. Fochi, S. Ranieri, A. Mazzanti, L. Bernardi, *Chem. Commun.* **2013**, *49*, 880-882.

The rotational strengths were calculated in both length and velocity representation, obtaining similar results (RMS difference < 5%) that ruled out large basis set incompleteness errors (BSSE).[20] The four different functionals provide similar results (Figure S6).

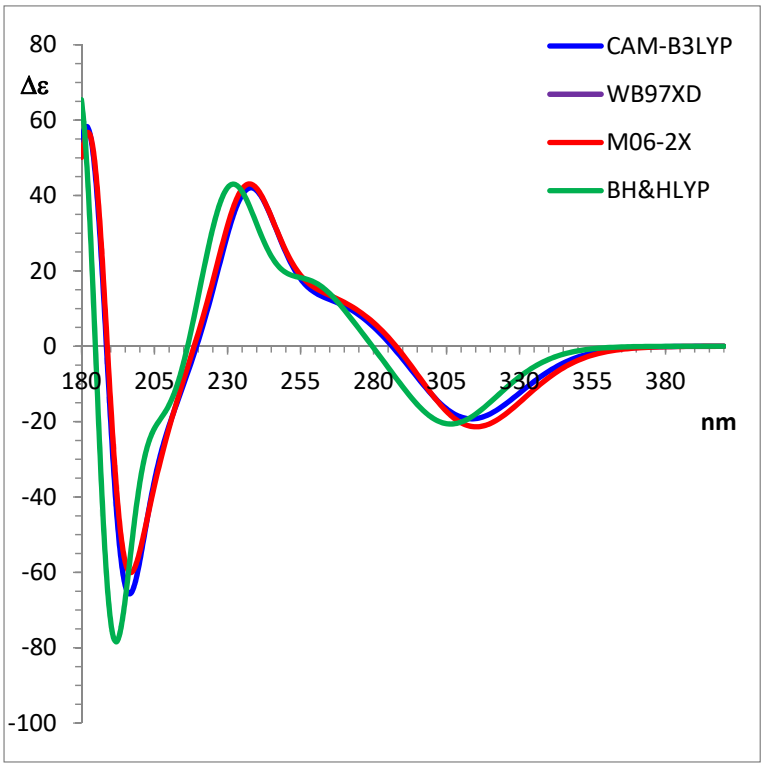


Fig. S6. TD-DFT simulated ECD spectra calculated for the same conformation of **3aa** assuming the *aR* absolute configuration, and using CAM-B3LYP, BH&HLYP, M06-2X, ωB97XD and the 6-311++G(2d,p) basis set. For each conformation, the first 50 excited states were calculated, and the spectrum was obtained using a 0.25 eV line half-width at half height.

The simulated spectra were vertically scaled to get the best match with the intensity of the experimental spectrum. Red-shifts were applied by comparison of the experimental with the simulated UV spectrum, (scaling factors: 0.40, 0.40, 0.40, 0.40; red shift: 16, 18, 16, 20 nm for CAM-B3LYP, ωB97XD, M06-2X and BH&HLYP, respectively). In all the cases the simulated spectra for the a*R* absolute configuration match very well the experimental spectrum (Figure S7).

[20]P. J. Stephens, D.M. McCann, F. J. Devlin, J.R. Cheeseman and M. J. Frisch, *J. Am. Chem. Soc.* **2004**, *126*, 7514-7521.

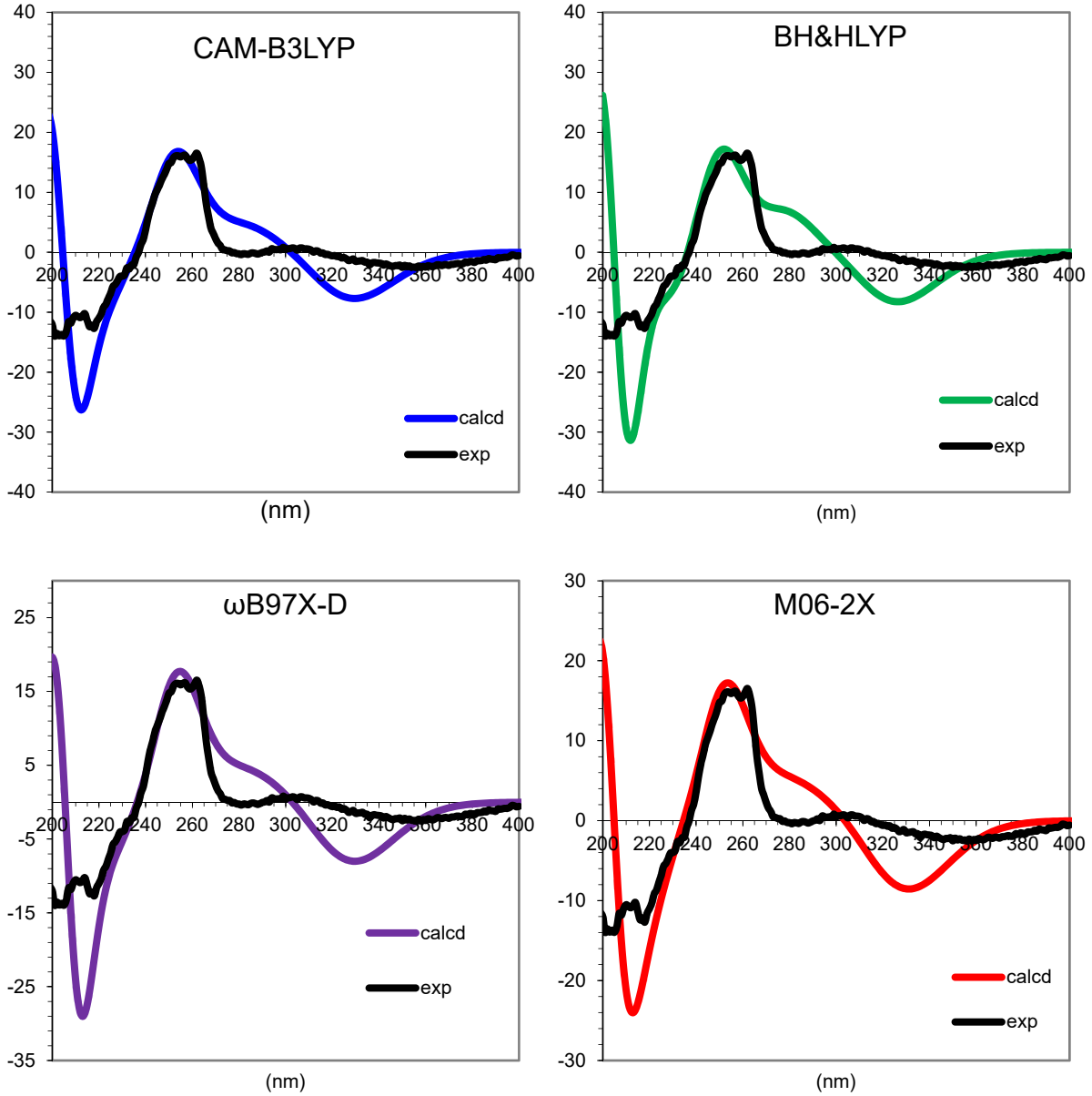
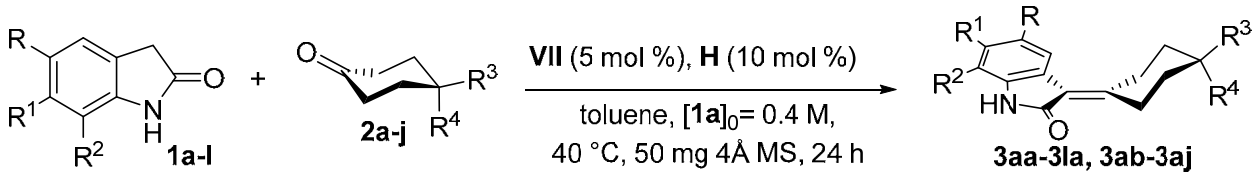


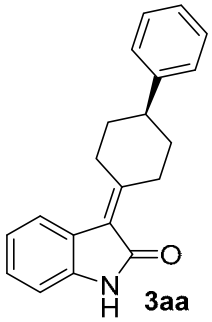
Fig. S7. Simulations of the experimental ECD spectrum of **3aa**. For each quadrant, the black line corresponds to the experimental spectrum. The colored lines correspond to the simulations obtained using the populations derived from PCM-B3LYP/6-311++G(2d,p) optimization. Simulated spectra were scaled and red-shifted for the best fit to the experimental spectrum.

General procedure for the catalytic Knoevenagel condensation of oxindoles and 4-substituted cyclohexanones



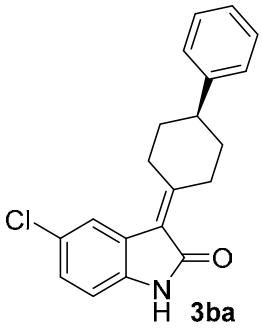
The reactions were carried out on a 0.2 mmol scale in shaded, 1.5 mL vials equipped with a magnetic stirrer. The catalyst, the acid, the oxindole, the ketone and the molecular sieves were placed in the vial before addition of toluene (500 µL) and the reaction was stirred at 40° C in a sand bath away from light for 24 hours. The solution was diluted in 15 ml of DCM/EtOAc 1/1 and flushed through a plug of silica (50 mL of DCM/EtOAc 1/1) to remove the catalyst using aluminium foils on the glassware to shield the light from the crude which, was immediately injected in the HPLC to check the enantiomeric ratio. The yield was determined via ^{1}H NMR directly from the crude mixture using 1,3,5-trimethoxybenzene as internal standard. Finally, the product was purified with flash column chromatography using the proper mixture of hexane and ethylacetate as eluent.

(*aR*)-3-(4-phenylcyclohexylidene)indolin-2-one (3aa)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3aa** was obtained in 87% yield (50.5 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20) and 13:87 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 22.4 min, $\tau_{\mathbf{Minor}}$ = 17.7 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{19}NNaO]^+$ 312.1359, found 312.1357 $[M+Na]^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.8 Hz, 1H), 8.08 (s, 1H), 7.27 – 7.21 (m, 2H), 7.18 – 7.13 (m, 3H), 6.93 (td, *J* = 7.7, 1.0 Hz, 1H), 6.82 – 6.77 (m, 1H), 4.81 – 4.56 (m, 1H), 3.51 (d, *J* = 14.3 Hz, 1H), 2.87 (tt, *J* = 12.0, 3.7 Hz, 1H), 2.46 (td, *J* = 13.6, 4.8 Hz, 1H), 2.29 – 2.08 (m, 3H), 1.84 – 1.62 (m, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 169.9, 162.6, 145.8, 139.4, 128.5, 127.8, 126.8, 126.3, 124.1, 123.8, 121.7, 120.6, 109.5, 43.6, 35.0, 34.7, 32.7, 29.6.

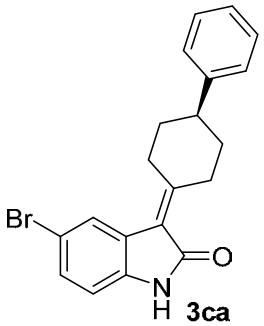
(*aR*)-5-chloro-3-(4-phenylcyclohexylidene)indolin-2-one (3ba)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ba** was obtained in 82% yield (53.0 mg, amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20) and 85:15 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 8.2 min, $\tau_{\mathbf{Minor}}$ = 11.0 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{19}ClNO]^+$ 324.1150, found 324.1149 $[M+H]^+$. **^{1}H NMR**

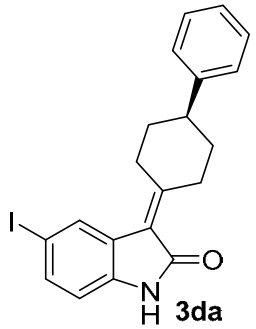
(300 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.64 (d, *J* = 2.0 Hz, 1H), 7.27 (m, 4H), 7.22 – 7.15 (m, 2H), 6.82 (d, *J* = 8.3 Hz, 1H), 4.66 (m, 1H), 2.93 (m, 1H), 2.56 (m, 1H), 2.21 – 2.00 (m, 3H), 1.67 (m, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.8, 162.2, 145.9, 141.9, 131.9, 128.4, 126.7, 12.1, 125.0, 122.2, 120.6, 119.6, 109.1, 42.6, 34.6, 34.3, 32.1, 28.6.

(*aR*)-5-bromo-3-(4-phenylcyclohexylidene)indolin-2-one (3ca)



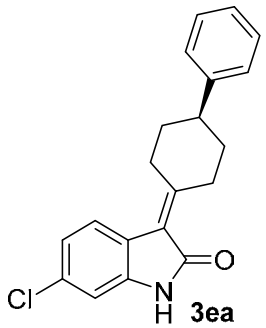
The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ca** was obtained in 85% yield (62.5.0 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20) and 82:18 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 8.3 min, τ_{Minor} = 11.1 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{19}BrNO]^+$ 368.0645, found 368.0644 $[M+H]^+$. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.62 (s, 1H), 7.75 (d, *J* = 1.9 Hz, 1H), 7.35 (dd, *J* = 8.2, 1.8 Hz, 1H), 7.31 – 7.23 (m, 4H), 7.21 – 7.16 (m, 1H), 6.79 (d, *J* = 8.3 Hz, 1H), 4.74 – 4.50 (m, 1H), 3.37 (s, 1H), 2.94 (tt, *J* = 11.9, 3.6 Hz, 1H), 2.67 – 2.52 (m, 1H), 2.25 (td, *J* = 13.5, 4.8 Hz, 1H), 2.14 (d, *J* = 12.7 Hz, 1H), 2.10 – 2.01 (m, 1H), 1.75 (qd, *J* = 12.8, 4.0 Hz, 1H), 1.62 (qd, *J* = 12.7, 3.9 Hz, 1H).**^{13}C NMR** (150 MHz, DMSO-d_6) δ 168.9, 163.9, 146.3, 140.1, 130.7, 128.8, 127.2, 126.5, 126.3, 125.8, 120.2, 113.2, 111.4, 42.9, 35.0, 34.6, 32.5, 29.1.

(*aR*)-5-iodo-3-(4-phenylcyclohexylidene)indolin-2-one (3da)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3da** was obtained in 78% yield (64.7 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20) and 91:9 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 8.2 min, $\tau_{\mathbf{Minor}}$ = 11.1 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{18}INNaO]^+$ 438.0331, found 438.0326 $[M+Na]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 10.61 (s, 1H), 7.88 (d, *J* = 1.6 Hz, 1H), 7.51 (dd, *J* = 8.1, 1.5 Hz, 1H), 7.33 – 7.18 (m, 5H), 6.68 (d, *J* = 8.1 Hz, 1H), 4.66 (d, *J* = 14.3 Hz, 1H), 3.32 – 3.24 (m, 1H), 3.04 – 2.85 (m, 1H), 2.61 – 2.52 (m, 1H), 2.28 – 2.01 (m, 3H), 1.80 – 1.58 (m, 2H). **^{13}C NMR** 13C NMR (151 MHz, DMSO-d_6) δ 167.6, 162.6, 145.1, 138.9, 129.5, 127.6, 125.9, 125.3, 125.1, 124.6, 118.9, 111.9, 110.2, 41.7, 33.8, 33.4, 31.3, 27.8.

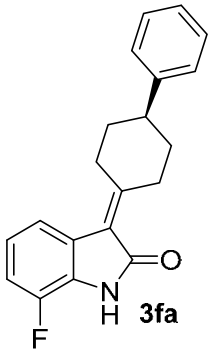
(*aR*)-6-chloro-3-(4-phenylcyclohexylidene)indolin-2-one (3ea)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ea** was obtained in 44% yield (28.6 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20) and 10:90 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 23.2 min, $\tau_{\mathbf{Minor}}$ = 19.7 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{19}ClNO]^+$ 324.1150, found 324.1149 $[M+H]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 10.62 (s, 1H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.34 – 7.23

(m, 4H), 7.22 – 7.14 (m, 1H), 6.97 (dd, *J* = 8.3, 2.1 Hz, 1H), 6.83 (d, *J* = 2.1 Hz, 1H), 4.65 (d, *J* = 14.2 Hz, 1H), 3.43 (overlapped with DMSO water, 1H), 3.04 – 2.82 (m, 1H), 2.57 (overlapped with DMSO, 1H), 2.28 – 2.00 (m, 3H), 1.81 – 1.54 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 168.8, 162.2, 145.9, 141.9, 131.9, 128.4, 126.7, 12.1, 125.0, 122.2, 120.6, 119.6, 109.1, 42.6, 34.6, 34.3, 32.1, 28.6.

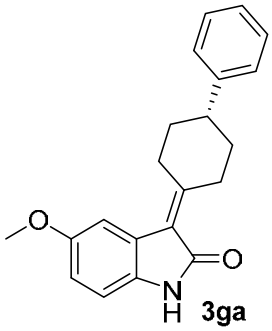
(*aR*)-7-fluoro-3-(4-phenylcyclohexylidene)indolin-2-one (3fa)



3fa

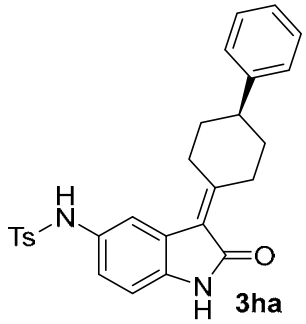
The reaction was carried out following the general procedure using catalyst **VII**. Compound **3fa** was obtained in 98% yield (60.4 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 95:5) and 79:21 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70:30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 11.9 min, τ_{Minor} = 16.0 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{19}FNO]^+$ 308.1445, found 308.1444 $[M+H]^+$. **^{1}H NMR** (400 MHz, DMSO-d_6) δ 10.95 (s, 1H), 7.52 (d, *J* = 8.0 Hz, 1H), 7.33 – 7.22 (m, 4H), 7.21 – 7.15 (m, 1H), 7.09 (ddd, *J* = 10.1, 8.4, 0.8 Hz, 1H), 6.94 (ddd, *J* = 8.4, 7.8, 5.3 Hz, 1H), 4.74 – 4.63 (m, 1H), 3.47 (d, *J* = 14.4 Hz, 1H), 2.95 (tt, *J* = 11.9, 3.6 Hz, 1H), 2.55 (dd, *J* = 13.6, 4.9 Hz, 1H), 2.24 (td, *J* = 13.4, 4.7 Hz, 1H), 2.18 – 2.00 (m, 2H), 1.68 (dqd, *J* = 41.2, 12.8, 3.8 Hz, 2H). **^{19}F NMR** (376 MHz, DMSO-d_6) -134.03 (dd, *J* = 10.2, 5.2 Hz). **^{13}C NMR** (100 MHz, DMSO-d_6) δ 169.1, 163.6, 148.0, 146.3, 145.6, 128.8, 128.1, 128.0, 127.2, 126.7, 126.7, 126.5, 122.0, 122.0, 120.6, 120.6, 120.3, 120.3, 115.0, 114.9, 43.0, 35.1, 34.8, 32.5, 29.0.

(*aS*)-5-methoxy-3-(4-phenylcyclohexylidene)indolin-2-one (3ga)



The reaction was carried out following the general procedure using catalyst **VIII**. Compound **3ga** was obtained in 68% yield (50.7 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20)and 17:83 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 17.8 min, $\tau_{\mathbf{Minor}}$ = 15.0 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{21}NNaO_2]^+$ 342.1465, found 342.1464 $[M+Na]^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.22 (s, 1H), 7.33 – 7.20 (m, 6H), 6.81 – 6.69 (m, 2H), 4.78 (d, *J* = 14.2 Hz, 1H), 3.80 (s, 3H), 3.54 (d, *J* = 14.2 Hz, 1H), 2.94 (m, 1H), 2.51 (m, 1H), 2.39 – 2.11 (m, 3H), 1.82 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 17031, 162.8, 155.0, 145.8, 133.4, 133.4, 128.5, 126.8, 126.3, 125.11, 121.0, 111.9 (double), 109.4, 56.,0 43.5, 34.9, 34.7, 32.6, 29.6.

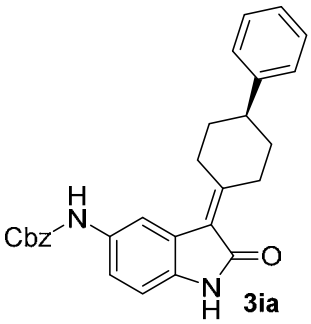
(*aR*)-4-methyl-N-(2-oxo-3-(4-phenylcyclohexylidene)indolin-5-yl)benzenesulfonamide (3ha)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ha** was obtained in 46% yield (42.6 mg, amorphous solid) by flash column chromatography (DCM:EtOAc = 70:30) and 81:19 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 30.0 min, $\tau_{\mathbf{Minor}}$ = 37.5 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{27}H_{26}N_2NaO_3S]^+$ 481.1556, found 481.1555 $[M+Na]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 10.41 (s, 1H), 9.73 (s, 1H), 7.59 – 7.52 (m, 2H), 7.35 – 7.12 (m, 8H), 6.87 (dd, *J* = 8.3, 1.9 Hz, 1H), 6.67 (d, *J* = 8.3 Hz, 1H), 4.62 (d, *J* = 13.9 Hz, 1H), 3.10 (d, *J* = 14.0 Hz, 1H),

3.01 – 2.80 (m, 1H), 2.41 (td, *J* = 13.7, 12.8, 3.9 Hz, 1H), 2.26 (s, 3H), 2.23 – 1.98 (m, 3H), 1.69 – 1.46 (m, 2H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ 168.8, 161.5, 145.8, 142.9, 137.9, 136.5, 130.6, 129.5, 128.4, 126.9, 126.7, 126.1, 123.5, 122.7, 120.3, 118.7, 109.3, 42.6, 34.7, 34.3, 31.7, 28.5, 20.9.

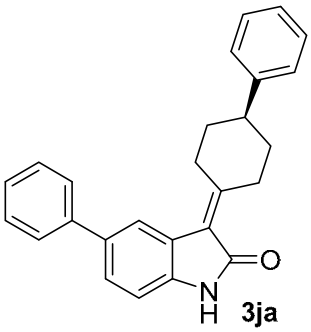
Benzyl-(*aR*)-(2-oxo-3-(4-phenylcyclohexylidene)indolin-5-yl)carbamate (3ia)



3ia

The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ia** was obtained in 11% yield (9.7 mg, white amorphous solid) by flash column chromatography (DCM:EtOAc = 70:30) and 20:80 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 22.4 min, τ_{Minor} = 17.7 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{28}H_{26}N_2NaO_3]^+$ 461.1836, found 461.1635 $[M+Na]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 10.36 (s, 1H), 9.54 (s, 1H), 7.86 (s, 1H), 7.50 – 7.04 (m, 12H), 6.73 (d, *J* = 8.3 Hz, 1H), 5.12 (s, 2H), 4.71 (d, *J* = 13.8 Hz, 1H), 3.41 (d, *J* = 12.1 Hz, 1H), 2.95 (t, *J* = 11.9 Hz, 1H), 2.37 – 1.95 (m, 4H), 1.83 – 1.54 (m, 2H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ 169.4, 161.2, 154.0, 146.4, 137.2, 128.8, 128.8, 128.4, 127.2, 123.9, 121.2, 109.4, 66.0, 43.1, 35.2, 34.7, 32.1, 29.0.

(*aR*)-5-phenyl-3-(4-phenylcyclohexylidene)indolin-2-one (3ja)

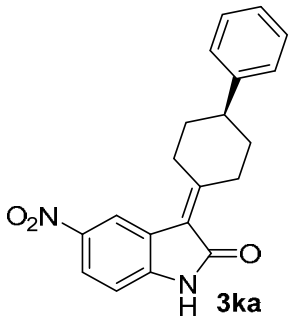


3ja

The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ja** was obtained in 67% yield (48.8 mg, amorphous solid) by flash column chromatography (hexane:EtOAc

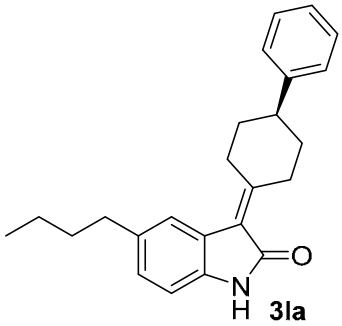
= 70:30) and 86:14 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70:30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 8.2 min, τ_{Minor} = 11.3 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{26}H_{24}NO]^+$ 366.1852, found 366.1851 $[M+H]^+$. **^{1}H NMR** (600 MHz, DMSO-d_6) δ 10.57 (s, 1H), 7.84 (d, *J* = 1.8 Hz, 1H), 7.66 – 7.57 (m, 2H), 7.51 – 7.37 (m, 3H), 7.37 – 7.24 (m, 5H), 7.18 (m, 1H), 6.92 (d, *J* = 8.1 Hz, 1H), 4.71 (m, 1H), 3.62 – 3.50 (m, 1H), 2.95 (m, 1H), 2.59 (m, 1H), 2.26 (m, 1H), 2.16 (m, 1H), 2.11 – 2.01 (m, 1H), 1.78 (m, 1H), 1.63 (m, 1H). **^{13}C NMR** (150 MHz, DMSO-d_6) δ 169.0, 161.6, 146.0, 140.9, 140.2, 133.4, 128.9, 128.4, 126.7 (double), 126.6, 126.5, 126.1, 124.0, 122.2, 120.5, 109.6, 42.6, 34.7, 34.2, 32.1, 28.6.

(*aR*)-5-nitro-3-(4-phenylcyclohexylidene)indolin-2-one (3ka)



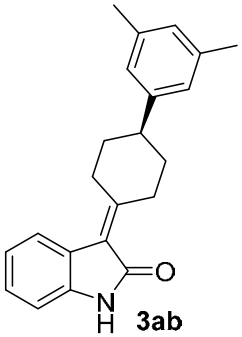
The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ka** was obtained in 43% yield (28.8 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 71:29 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 50:50, flow rate 0.6 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 9.2 min, τ_{Minor} = 12.2 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{18}N_2NaO_3]^+$ 357.1210, found 357.1208 $[M+Na]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 11.23 (s, 1H), 8.40 (d, *J* = 2.2 Hz, 1H), 8.16 (dd, *J* = 8.7, 2.2 Hz, 1H), 7.33 – 7.24 (m, 4H), 7.19 (ddd, *J* = 6.9, 5.7, 2.5 Hz, 1H), 7.01 (d, *J* = 8.7 Hz, 1H), 4.62 (d, *J* = 14.6 Hz, 1H), 3.51 – 3.39 (d, *J* = 14.6 Hz, 1H), 3.05 – 2.88 (m, 1H), 2.68 (m, 1H), 2.43 – 2.01 (m, 3H), 1.73 (m, 2H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ 168.9, 165.9, 146.4, 145.8, 141.5, 128.4, 126.8, 126.1, 124.8, 123.5, 119.0, 118.7, 109.2, 42.28, 34.4, 34.0, 32.2, 28.9.

(*aR*)-5-butyl-3-(4-phenylcyclohexylidene)indolin-2-one (3la)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3la** was obtained in 65% yield (35.3 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 80:20) and 82:18 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak IC column: hexane/*i*-PrOH 90:10, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 16.5 min, $\tau_{\mathbf{Minor}}$ = 18.2 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{24}H_{27}NNaO]^+$ 368.1985, found 368.1985 $[M+Na]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 10.36 (s, 1H), 7.52 – 7.41 (m, 1H), 7.31 – 7.16 (m, 5H), 6.99 (dd, *J* = 7.9, 1.5 Hz, 1H), 6.73 (d, *J* = 7.8 Hz, 1H), 4.72 (d, *J* = 13.9 Hz, 1H), 3.49 (d, *J* = 14.4 Hz, 1H), 2.92 (td, *J* = 12.0, 6.0 Hz, 1H), 2.51 (p, *J* = 1.9 Hz, 3H), 2.25 – 2.00 (m, 3H), 1.80 – 1.48 (m, 4H), 1.30 (q, *J* = 7.4 Hz, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ 169.52, 160.67, 146.47, 138.98, 135.26, 128.82, 128.04, 127.20, 126.51, 124.21, 123.87, 121.21, 109.38, 43.16, 35.33, 35.23, 34.73, 34.29, 32.36, 28.91, 22.21, 14.26.

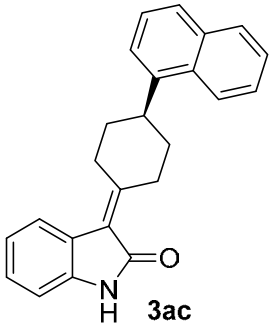
(*aR*)-3-(4-(3,5-dimethylphenyl)cyclohexylidene)indolin-2-one (3ab)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ab** was obtained in 91% yield (57.7 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 83:17 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 50/50, flow rate 0.6 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 9.6 min, $\tau_{\mathbf{Minor}}$ = 12.9 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{22}H_{24}NO]^+$ 318.1852, found

318.1853 [M+H]$^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.33 (s, 1H), 7.67 – 7.61 (m, 1H), 7.18 (td, *J* = 7.6, 1.1 Hz, 1H), 6.99 (td, *J* = 7.7, 1.1 Hz, 1H), 6.88 (d, *J* = 1.1 Hz, 1H), 6.85 (s, 3H), 4.82 – 4.71 (m, 1H), 3.56 (d, *J* = 14.2 Hz, 1H), 2.87 (ddd, *J* = 12.0, 8.2, 3.7 Hz, 1H), 2.50 (td, *J* = 13.7, 4.8 Hz, 1H), 2.29 (d, *J* = 0.7 Hz, 6H), 2.26 – 2.11 (m, 3H), 1.90 – 1.68 (m, 2H). **^{13}C NMR** ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.0, 162.9, 145.8, 139.4, 137.9, 127.9, 127.7, 124.7, 124.1, 123.8, 121.7, 120.6, 109.5, 43.5, 35.1, 34.8, 32.9, 29.8, 21.3.

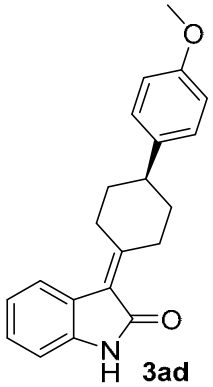
(*aR*)-3-(4-(naphthalen-1-yl)cyclohexylidene)indolin-2-one (3ac)



3ac

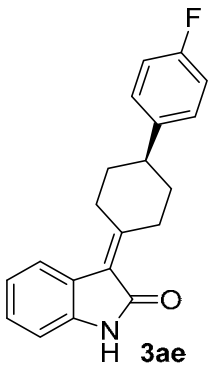
The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ac** was obtained in 67% yield (45.5 mg, white amorphous solid) by flash column chromatography (DCM:EtOAc = 90:10) and 15:85 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 28.5 min, τ_{Minor} = 20.1 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{24}H_{21}NNaO]^+$ 362.1521, found 362.1515 [M+Na]$^+$. **^{1}H NMR** (400 MHz, DMOS-d_6) δ 10.48 (s, 1H, NH), 8.3 (d, *J* = 8.9 Hz, 1H), 7.93 (dd, *J* = 8.1, 1.3 Hz, 1H), 7.78 (d, *J* = 8.1 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), (m, 1H), 7.62-7.57 (m, 1H), 7.56-7.50 (m, 1H), 7.48-7.39 (m, 2H), 7.18 (td, *J* = 7.7, 1.1 Hz, 1H), 6.95 (td, *J* = 7.6, 1.1 Hz, 1H), 6.84 (dd, *J* = 7.7, 0.8 Hz, 1H), 4.79 (bd, *J* = 14.7 Hz, 1H), 3.82 (tt, *J* = 11.7, 2.9 Hz, 1H), 3.55 (bd, *J* = 14.5 Hz), 2.73 (td, *J* = 13.4, 4.9 Hz, 1H), (2.42 (td, *J* = 13.2, 4.3 Hz, 1H), 2.29 – 2.09 (m, 1H), 1.91 – 1.64 (m, 2H). **^{13}C NMR** (75 MHz, DMOS-d_6) δ 168.9, 160.9, 141.9, 140.6, 133.5, 130.9, 128.8, 127.8, 126.4, 126.0, 125.7, 125.5, 123.8, 123.4, 123.2, 122.3, 121.0, 120.6, 109.2, 37.3, 34.2, 34.0, 32.0, 28.6.

(*aR*)-3-(4-(4-methoxyphenyl)cyclohexylidene)indolin-2-one (3ad)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ad** was obtained in 90% yield (57.5 mg, white amorphous solid) and 80:20 e.r. The crude mixture was purified by flash column chromatography (hexane:EtOAc = 70:30). The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 23.3 min, $\tau_{\mathbf{Minor}}$ = 36.9 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{21}H_{21}NNaO_2]^+$ 342.1470, found 342.1464 $[M+Na]^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 7.90 (s, 1H), 7.67 – 7.62 (m, 1H), 7.23 – 7.11 (m, 3H), 7.00 (td, *J* = 7.7, 1.1 Hz, 1H), 6.89 – 6.82 (m, 3H), 4.82 – 4.70 (m, 1H), 3.79 (s, 3H), 3.61 – 3.50 (m, 1H), 2.90 (tt, *J* = 12.0, 3.7 Hz, 1H), 2.51 (td, *J* = 13.7, 4.8 Hz, 1H), 2.23 (dddd, *J* = 21.6, 14.3, 12.2, 5.9 Hz, 3H), 1.87 – 1.69 (m, 2H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 169.7, 162.6, 158.0, 139.3, 138.0, 127.7, 127.6, 124.1, 123.8, 121.7, 120.5, 113.9, 109.4, 55.3, 42.7, 35.2, 35.0, 32.8, 31.6, 29.7, 22.6, 14.1.

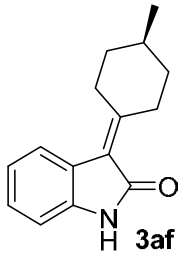
(*aR*)-3-(4-(4-fluorophenyl)cyclohexylidene)indolin-2-one (3ae)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ae** was obtained in 89% yield (54.7 mg, amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 18:82 e.r.. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column:

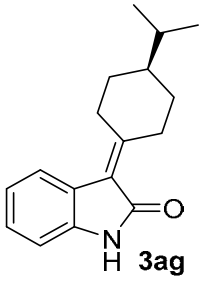
hexane/*i*-PrOH 70:30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 31.4 min, τ_{Minor} = 22.3 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{18}FNNaO]^+$ 330.1265, found 330.1263 $[M+Na]^+$. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.41 (s, 1H), 7.63 (dd, *J* = 7.9, 1.1 Hz, 1H), 7.24 – 7.11 (m, 3H), 7.05 – 6.94 (m, 3H), 6.92 – 6.83 (m, 1H), 4.88 – 4.70 (m, 1H), 3.64 – 3.51 (m, 1H), 2.93 (m, 1H), 2.51 (m, 1H), 2.34 – 2.11 (m, 2H), 1.88 – 1.62 (m, 3H). **^{19}F NMR** (286 MHz, $CDCl_3$) δ -117.1. **^{13}C NMR** (75 MHz, $CDCl_3$) δ 170.0, 163.0, 162.0, 159.8, 141.5, 141.4, 139.5, 128.2, 128.0, 127.8, 124.0, 123.8, 121.7, 120.8, 115.3, 115.0, 109.6, 42.8, 35.1, 34.9, 32.6, 29.6.

(*aR*)-3-(4-methylcyclohexylidene)indolin-2-one (3af)



The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ba** was obtained in 90% yield (40.8 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 75:25 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 14.4 min, τ_{Minor} = 18.3 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{15}H_{18}NO]^+$ 228.1383, found 228.1381 $[M+H]^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.58 (s, 1H), 7.65 – 7.58 (m, 1H), 7.17 (td, *J* = 7.7, 1.1 Hz, 1H), 6.98 (td, *J* = 7.7, 1.2 Hz, 1H), 6.91 – 6.82 (m, 1H), 4.49 (dt, *J* = 14.2, 2.0 Hz, 1H), 3.46 – 3.33 (m, 1H), 2.47 – 2.18 (m, 2H), 2.00 (ddtd, *J* = 18.4, 10.9, 4.0, 2.3 Hz, 2H), 1.28 (dtdd, *J* = 23.6, 12.7, 10.9, 4.0 Hz, 3H), 0.96 (d, *J* = 6.6 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 170.20, 164.21, 139.41, 127.55, 124.19, 123.73, 121.55, 120.27, 109.48, 36.00, 35.63, 32.36, 31.72, 29.28, 21.57.

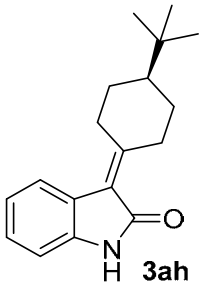
(*aR*)-3-(4-isopropylcyclohexylidene)indolin-2-one (3ag)



3ag

The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ag** was obtained in 85% yield (38.2 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 32:68 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 30.4 min, $\tau_{\mathbf{Minor}}$ = 26.5 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{17}H_{22}NO]^+$ 256.1696, found 256.1696 $[M+H]^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.43 (s, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.16 (td, *J* = 7.7, 1.1 Hz, 1H), 6.98 (td, *J* = 7.7, 1.2 Hz, 1H), 6.86 (ddd, *J* = 7.7, 1.2, 0.5 Hz, 1H), 4.57 – 4.41 (m, 1H), 3.47 – 3.38 (m, 1H), 2.30 (dddd, *J* = 41.2, 14.1, 12.1, 4.9 Hz, 2H), 2.09 – 1.94 (m, 2H), 1.63 – 1.18 (m, 4H), 0.90 (d, *J* = 6.5 Hz, 6H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 170.13, 164.67, 164.59, 139.39, 127.51, 124.23, 121.54, 120.07, 109.44, 42.99, 32.60, 32.31, 30.74, 30.39, 29.38, 19.90.

(*aR*)-3-(4-(*tert*-butyl)cyclohexylidene)indolin-2-one (3ah)

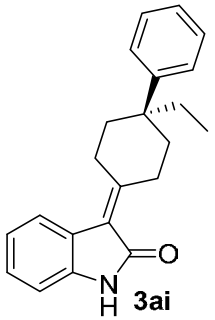


3ah

The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ah** was obtained in 86% yield (46.3 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 14:86 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 70/30, flow rate 0.8 mL/min, 25 °C, λ = 254 nm: $\tau_{\mathbf{Major}}$ = 19.5 min, $\tau_{\mathbf{Minor}}$ = 14.5 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{18}H_{24}NO]^+$ 270.1852, found 270.1853 $[M+Na]^+$. **^{1}H NMR** (300 MHz, $CDCl_3$) δ 8.51 (s, 1H), 7.60 (dd, *J* = 7.6, 1.0 Hz, 1H), 7.17 (td, *J* = 7.7, 1.1 Hz, 1H), 6.98 (td, *J* = 7.7, 1.1 Hz, 1H), 6.90 – 6.83 (m, 1H), 4.49 (dd, *J* = 14.5, 2.0 Hz, 1H),

3.44 (dd, *J* = 14.4, 2.3 Hz, 1H), 2.44 – 2.19 (m, 2H), 2.13 – 1.97 (m, 2H), 1.46 – 1.24 (m, 3H), 0.89 (s, 9H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 170.16, 164.53, 139.40, 127.50, 124.23, 123.70, 121.53, 120.02, 109.45, 46.93, 32.92, 32.62, 29.55, 28.30, 27.96, 27.46.

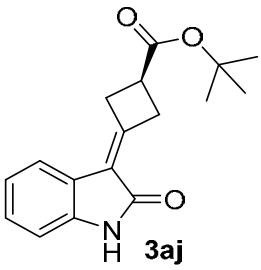
(*aR*)-3-(4-ethyl-4-phenylcyclohexylidene)indolin-2-one (3ai)



3ai

The reaction was carried out following the general procedure using catalyst **VII**. Compound **3ai** was obtained in 78% yield (49.5 mg, white amorphous solid) by flash column chromatography (hexane:EtOAc = 70:30) and 63:37. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 50:50, flow rate 0.6 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 49.9 min, τ_{Minor} = 62.2 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{22}H_{23}NNaO]^+$ 340.1672, found 340.1671 $[M+Na]^+$. **^{1}H NMR** (300 MHz, DMSO-d_6) δ 10.40 (s, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.46 – 7.33 (m, 4H), 7.27–7.06 (m, 2H), 6.95-6.85 (m, 1H), 6.82 – 6.74 (m, 1H), 3.88 (dt, *J* = 15.5, 5.1 Hz, 1H), 3.08 (dt, *J* = 15.4, 5.0 Hz, 1H), 2.70-2.53 (m, 1H), 2.43 – 2.22 (m, 2H), 1.76 (dddd, *J* = 28.0, 14.2, 10.4, 4.0 Hz, 3H), 1.59 (q, *J* = 7.3 Hz, 2H), 0.54 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (75 MHz, DMSO-d_6) δ 169.25, 161.79, 145.46, 140.91, 128.74, 128.12, 127.13, 126.08, 124.10, 123.77, 121.34, 120.81, 109.57, 35.85, 35.77, 35.51, 28.86, 25.38, 8.62.

(*aR*)-*tert*-butyl 3-(2-oxoindolin-3-ylidene)cyclobutane-1-carboxylate (3aj)

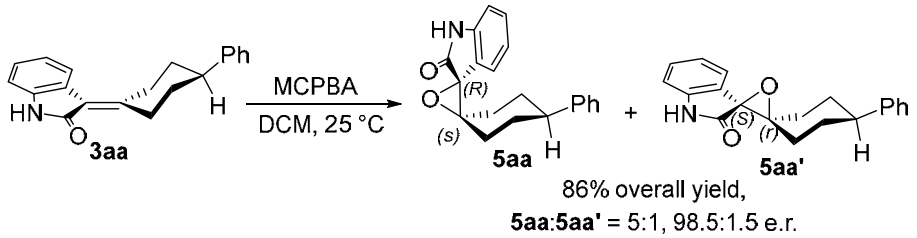


3aj

The reaction was carried out following the general procedure using catalyst **VII**. Compound **3aj** was obtained in 19% yield (12.9 mg, white amorphous solid) by flash column chromatography

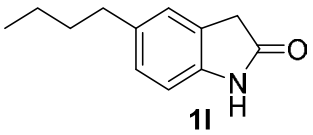
(hexane:EtOAc = 60:40) and 56:44 e.r. The e.r. was determined by HPLC analysis on a Daicel Chiralpak AD-H column: hexane/*i*-PrOH 50:50, flow rate 0.6 mL/min, 25 °C, λ = 254 nm: τ_{Major} = 9.1 min, τ_{Minor} = 17.6 min. HRMS-ESI-ORBITRAP (+): calculated for $[C_{17}H_{19}NNaO_3]^+$ 308.1257, found 308.1256 $[M+Na]^+$. **^{1}H NMR** (400 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.18 (dd, $J_1 = J_2$ = 7.6 Hz, 2H), 7.05 – 6.96 (m, 1H), 6.85 (ddd, *J* = 7.4, 0.9 Hz, 1H), 3.76 – 3.64 (m, 1H), 3.60 – 3.47 (m, 2H), 3.47 – 3.36 (m, 2H), 1.49 (s, *J* = 0.5 Hz, 9H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 173.4, 168.4, 156.4, 139.7, 128.1, 123.2, 122.1, 121.9, 121.4, 109.6, 81.0, 37.6, 36.8, 35.9, 28.1.

(1*s*,3'*R*)-4-phenyldispiro[cyclohexane-1,2'-oxirane-3',3''-indolin]-2''-one (5aa) and (1*r*,3'*S*)-4-phenyldispiro[cyclohexane-1,2'-oxirane-3',3''-indolin]-2''-one (5aa')



In an ordinary vial containing product **3aa** (0.1 mmol, 1 equiv, 28.9 mg) and *m*-CPBA (0.11 mmol, 1.1 equiv, 24.7 mg of commercialy available 77% *m*-CPBA) was added DCM (5.8 mL, 0.017 M) and the solution was left in an ice bath under magnetic stirring. After 2 hours, the crude was diluted with more DCM and quenched with a $NaHCO_3$ aqueous solution. After 2 extractions and removal of water with anhydrous $MgSO_4$, flash column chromatography (hexane:EtOAc 70:30) afforded 27 mg of title compound (70% isolated yield, 23 mg of white solid) as a 5:1 mixture of diastereoisomers. HPLC analysis on a Daicel Chiralpak AD-H column (hexane/*i*-PrOH 40/60, flow rate 0.3 mL/min, 25° C, λ = 254 nm) showed a 98.5:1.5 e.r. on both diastereoisomers. HRMS-ESI-ORBITRAP (+): calculated for $[C_{20}H_{19}NNaO_2]^+$ 328.1308, found 328.1307 $[M+Na]^+$. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 8.78 (bs, 1H), 7.37 – 7.18 (m, 7H), 7.04 (ddd, *J* = 7.6, 1.0 Hz, 1H), 6.97 (d, *J* = 8.0, 1H), 2.89 (m, 1H), 2.71 (m, 1H), 2.24 – 1.67 (m, 7H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 175.4 (double), 146.1, 145.4, 142.1, 142.0, 129.7 (double), 128.5, 1283, 126.8, 126.6, 126.3, 126.2, 124.9, 124.5, 123.4, 123.3, 122.3, 122.1, 110.7, 110.6, 71.8, 70.5, 65.6, 64.7, 43.7, 43.0, 33.2, 32.9, 32.1, 31.9, 30.4, 30.2, 29.7, 27.5.

5-butyloxindole (1l)



1l

The reaction was carried out following the literature procedure.[21] 5-butylisatin (15 mmol, 1 equiv) was placed in a 100 mL round flask and suspended in MeOH (37.5 mL, 0.4 M) before adding hydrazine (30.15 mmol, 2.6 ml of 55% solution in water, 2 equiv). The solution was left refluxing (2 to 3 hours) under magnetic stirring until the formation of a precipitate is observed, then cooled to room temperature. The precipitate was filtered on a gooch funnel, washed with water, cold MeOH and cold Et_2O to afford the pure hydrazone that was added to a freshly prepared solution of EtONa in EtOH (3.7 equiv of metallic Na dissolved in EtOH so that the hydrazone is 0.4M). This new solution was once again heated to reflux until the reagent disappeared (TLC monitoring), then it was cooled and quenched with 10% HCl. The crude was now extracted with DCM, made anhydrous over $MgSO_4$ and purified by either flash column chromatography or crystallization to obtain the pure oxindole. The crude mixture was purified by flash column chromatography (hexane:EtOAc = 75:25) and the title compound was obtained in 63% yield (2.0 g, yellow solid). HRMS-ESI-ORBITRAP (+): calculated for $[C_{12}H_{15}NNaO]^+$ 212.1051, found 212.1049 $[M+Na]^+$. **^{1}H NMR** (300 MHz, Chloroform-*d*) δ 9.27 (s, 1H), 7.13 – 6.94 (m, 2H), 6.81 (d, *J* = 7.9 Hz, 1H), 3.51 (s, 2H), 2.75 – 2.42 (m, 2H), 1.69 – 1.45 (m, 2H), 1.45 – 1.20 (m, 2H), 0.92 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (75 MHz, $CDCl_3$) δ 178.3, 140.3, 137.0, 127.6, 125.3, 124.6, 109.5, 36.4, 35.3, 34.0, 22.2, 13.9.

[21] (a) S. Crotti, G. Belletti, N. Di Iorio, E. Marotta, A. Mazzanti, P. Righi, G. Bencivenni *RSC Adv*., **2018**, *8*, 33451. (b) S. Crotti, N. Di Iorio, A. Mazzanti, P. Righi, G. Bencivenni *J. Org. Chem*. **2018**, *83*, 12440.

Computational details

All of the quantum-chemical computations were performed using the Gaussian 16 package.[22] Preliminary computational studies on the iminium ions and the transition states for the nucleophilic addition of oxindole to the iminium ion were performed using at the B3LYP/6-31G(d) level of theory. The B3LYP/6-31G(d) method has been widely used to model organocatalytic reactions.[23] Some issues associated to the B3LYP in accounting for dispersion have been recently pointed out. However, Goodman compared various density functionals and found that for transition-structure geometry optimizations, B3LYP is slightly less accurate than newer, dispersion-inclusive functionals, which are more computationally demanding.[24]

After the preliminary studies, the computational studies examining the main points of the reaction paths leading to major (a*S*)- and minor (a*R*)-product were studied at 313 K using the metahybrid DFT functional M06-2X[25,26] together with the universal continuum solvation model (SMD). The thermal corrections evaluated on the optimized geometries at 313 K from the unscaled vibrational frequencies[27] with the M06-2X/6-31G(d)/SMD(toluene) level of theory were then added to the M06-2X/6-311++G(2d,p)/SMD(toluene) electronic energies to obtain the corrected free energies.[24,28,29] The free energy corrections were calculated using Truhlar's quasi-harmonic approximation[30] as implemented in the GoodVibes program.[31]

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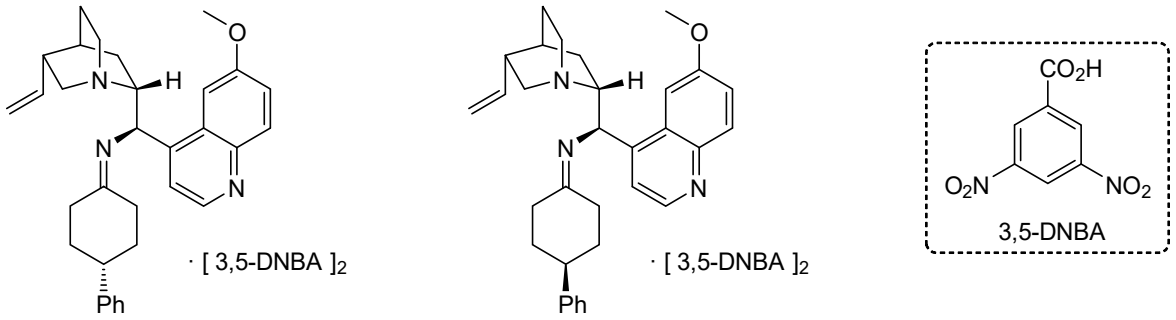
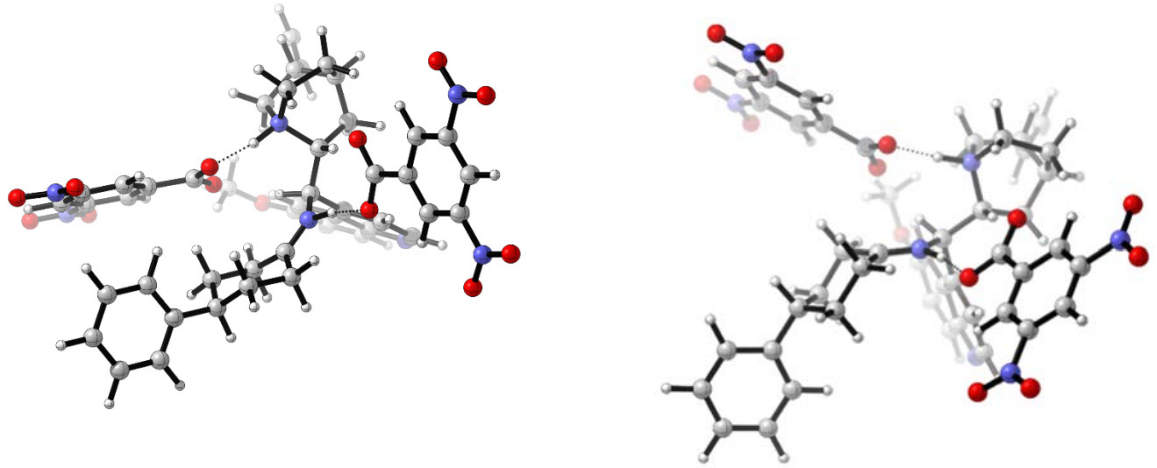
Iminium Ion

The reaction of the 9-*epi*-9-amminoquinidine (9-*epi*-NH_2-QDA) catalyst with 4-phenylcyclohexanone, in the presence of 3,5-dinitrobenzoic acid, affords the two diastereoisomeric iminium ions (*aR*)- and (*aS*)-**A**.



(*aR*)-**A** (*aS*)-**A**

Previous extensive conformational analysis on cinchona alkaloids and their iminium derivatives[28, 29] showed that the cinchona alkaloids prefer to adopt the *anti-open* conformation which was the only one considered in the following calculations. A relaxed potential energy surface (PES) scan at the semiempirical PM6 level was performed on both iminium ions (*aR*)- and (*aS*)-**A** by the systematic variation of the C9-N bond dihedral angle. All the structures within 5 kcal/mol from the one with the lowest energy were reoptimized at the B3LYP/6-31G(d) level. A total of six conformations were located for the iminium ion (*aR*)-**A** and five for (*aS*)-**A** which accounted for a cumulative distribution of ca. 80 : 20 in favor of (*aR*)-**A**. The lowest energy conformation located for both (*aR*)-**A** and (*aS*)-**A** are shown in Fig. S7



(a*R*)-**A**: G°: 0.0 (a*S*)-**A**: G°: 0.8

Fig. S7.[32] Equilibrium geometries for (a*R*)-iminium ion (left) and (a*S*)-iminium ion (right). The geometries were obtained at B3LYP/6-311+G(2d,p)-PCM(toluene)//B3LYP/6-31G(d) level of theory.

[32] All 3D representations were obtained using CYLview visualization software: CYLview, 1.0b; Legault, C. Y., Université de Sherbrooke, 2009 (http://www.cylview.org)

Transition states for the nucleophilic addition of oxindole to the iminium ion

We then focused our attention to the search transition states for the nucleophilic addition step of the oxindole to the lowest energy conformation of the iminium ions (*aR*)- and (*aS*)-**A**. Sixteen starting points were selected for this search, which are the result of the variation of four structural motifs: (i) axial configuration (*aR*) or (*aS*) of the starting iminium ion with the phenyl group in an equatorial disposition; (ii) same as (i) but with the phenyl in an axial disposition; (iii) heterotopic *Re* or *Si* face of the starting oxindole; (iv) heterotopic *re* or *si* face[33] of the iminium ion. This search resulted in the location of eight transition state structures (**TS-1a** – **TS-1h**). Selected data for these eight transition state geometries are reported in Table S6.

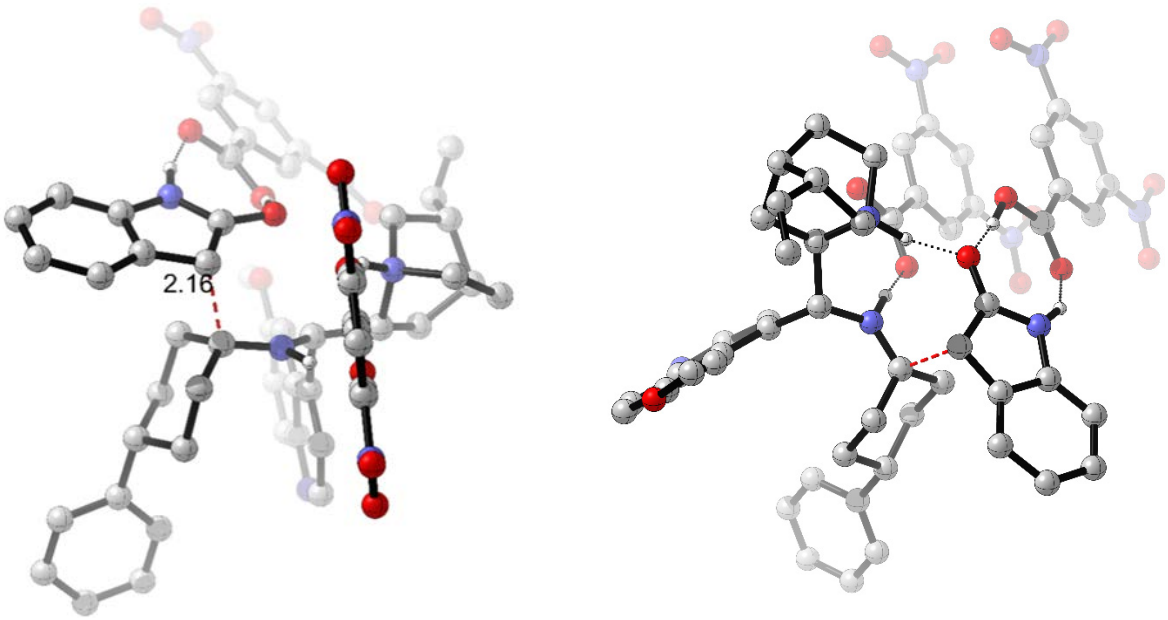
Table S6

Entry	E[a] [kcal/mol]	qh-G(T)[b] [kcal/mol]
TS-1a	0.0	0.0
TS-1b	1.1	2.0
TS-1c	4.0	4.1
TS-1d	5.0	6.3
TS-1e	5.0	6.3
TS-1f	7.2	7.4
TS-1g	11.1	11.4
TS-1h	11.6	11.3

a) Relative electronic energy at the B3LYP/6-311+G(2d,p)/PCM(toluene) level of theory. b) relative free energy calculated from Gaussian results at the B3LYP/6-31G(d) level of theory using Truhlar's quasi-harmonic approximation as implemented[30] in the GoodVibes program[31]

The two lower energy transition state structures **TS-1a** and **TS-1b** were further refined at the M06-2X/6-311++G(2d,p)/SMD(toluene)//M06-2X/6-31G(d)/SMD(toluene) level of theory and are shown in Fig. S8. **TS-1a** is the attack from the *Re* face of the oxindole to the *re* face of the iminium ion (*aS*)-**A** while **TS-1b** is the attack of the *Si* face of the oxindole to the *re* face of the same iminium ion (*aS*)-**A**. All the located transition states showed that the oxindole unit binds via hydrogen bonding of its amidic moiety to a carboxylic acid unit. A feature that is kept throughout the entire reaction path.

[33] E. L. Eliel, S. H. Wilen in *Stereochemistry of Organic Compounds*, Wiley 1994, p. 484



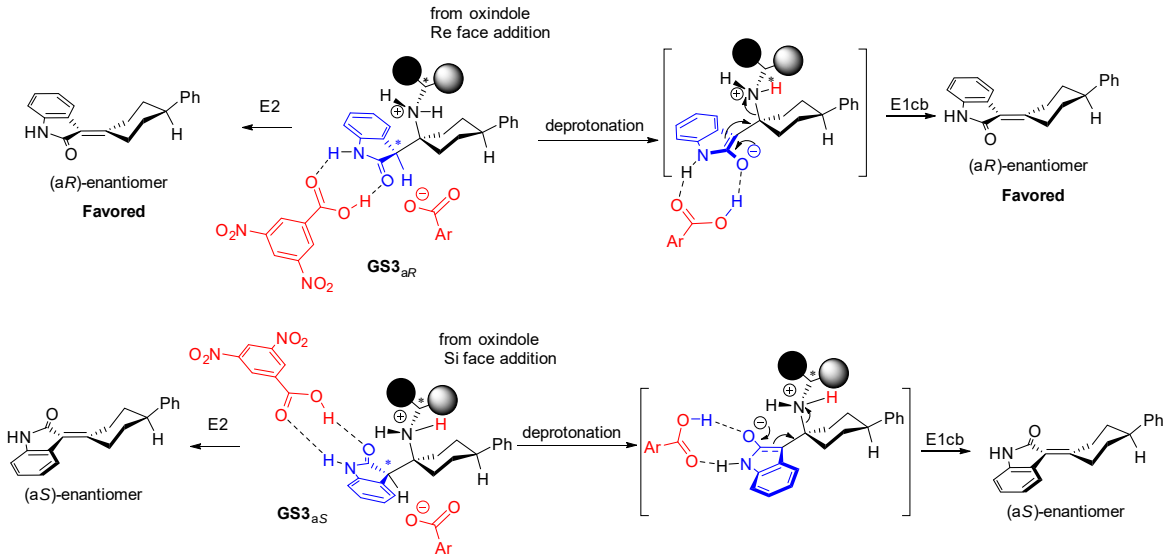
TS-1a: qh-G_{313}: 0.0
Im. freq.: -242.66 cm^{-1}

TS-1b: qh-G_{313}: 1.2
Im. freq.: -154.25 cm^{-1}

Fig. S8. Transition state geometries leading to (a*R*)-product (left) and to the (a*S*)-product (right). The geometries obtained at 313 K with the M06-2X/6-311++G(2d,p)/SMD(toluene)//M06-2X/6-31G(d)/SMD(toluene) level of theory. qh-G_{313}, relative Truhlar quasi-harmonic corrected free energy [kcal/mol] at 313 K with a cutoff of 100 cm^{-1}

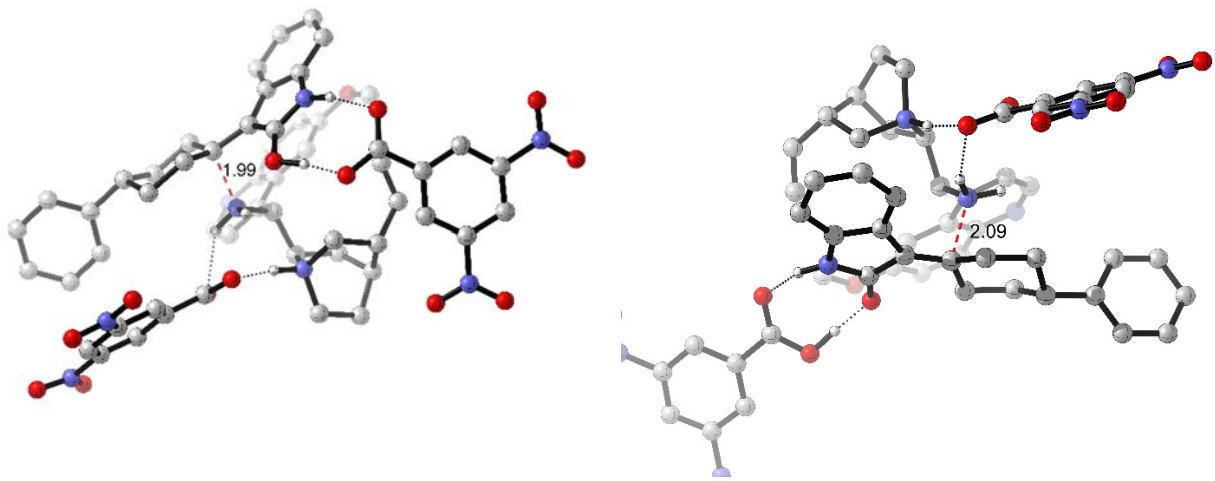
Transition states for the final E1cb elimination

For the final elimination step, in which the atropisomeric double bond is formed and the product is released from the catalyst, we investigated both the E2 and the E1cb hypothesis. Both mechanisms require the preliminary protonation of the amine nitrogen to create a good leaving group.



Scheme S1. Alternative pathways for the final elimination to the products: E2 (left) and E1cb (right).

The geometries for the two E1cb transition states were located and were found to favor the transition state leading to (a*R*)-product by 4.6 kcal/mol (Figure S9).

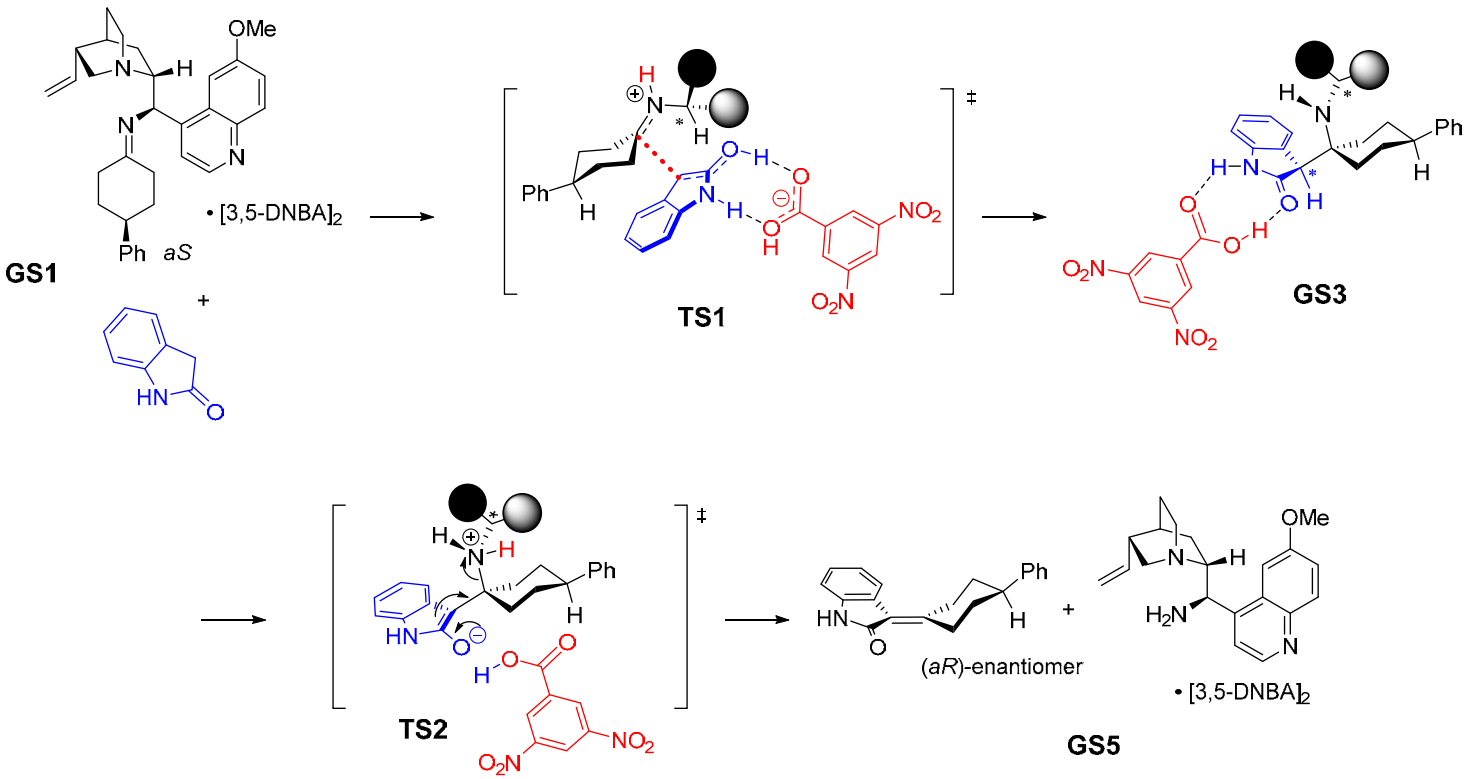


TS-2a: qh-G_{313}: 0.0
Im. freq.: -240.53 cm^{-1}

TS-2b: qh-G_{313}: 4.6
Im. freq.: -225.27 cm^{-1}

Fig. S9. Transition state geometries leading to the major (a*R*)-product (left) and to the minor (a*S*)-product (right). The geometries obtained at 313 K with the M06-2X/6-311++G(2d,p)/SMD(toluene)//M06-2X/6-31G(d)/SMD(toluene) level of theory. qh-G_{313}, relative Truhlar quasi-harmonic corrected free energy [kcal/mol] at 313 K with a cutoff of 100 cm^{-1}

The transition state for the E2 elimination to the favored (a*R*)-product could also be located and was found to be ca. 15 kcal/mol higher than the corresponding E1cb step.



Scheme S2. Main steps in the proposed reaction path for the asymmetric enantioselective Knoevenagel condensation (aEKC)

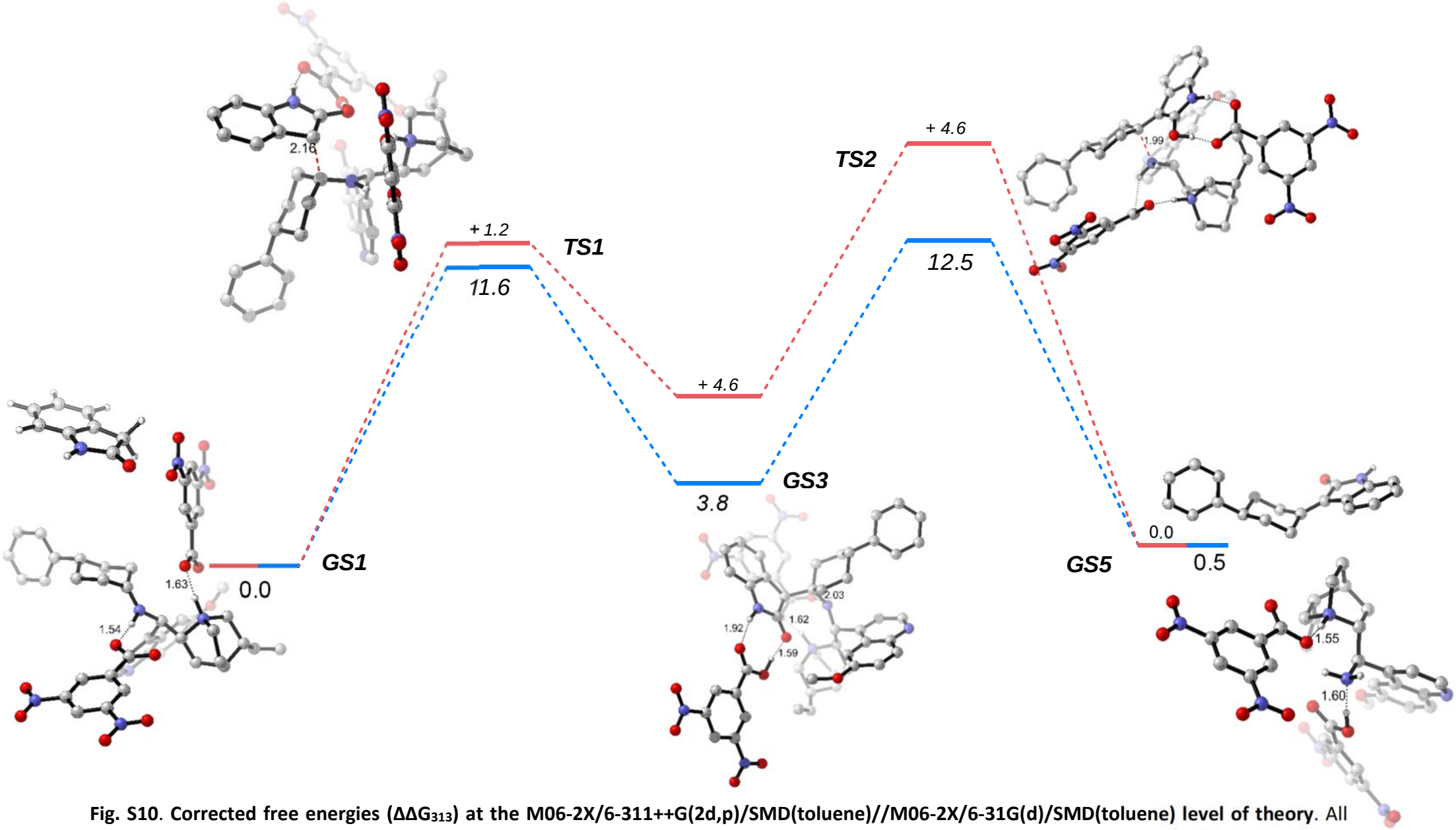


Fig. S10. **Corrected free energies ($\Delta\Delta G_{313}$) at the M06-2X/6-311++G(2d,p)/SMD(toluene)//M06-2X/6-31G(d)/SMD(toluene) level of theory**. All values are in kcal/mol. Blue: reaction path to the major (*aR*)-product; red: reaction path to the minor (*aS*)-product. Values for the red path are expressed relative to the corresponding values of the blue path. 3D representations refer to structures of the reaction pathway to the major (a*R*)-product

(a*S*)-iminium ion

E_{313}: -3140.587836
qh-G_{313}: -3139.77765

C	1.802369	-4.332265	-1.033060
C	0.916216	-3.385578	-1.867473
C	-1.707960	-6.866436	1.021480
C	-1.113626	-5.678897	1.092161
C	1.415247	-0.253119	2.781041
C	-0.706976	-1.285542	3.287153
C	-0.353590	-1.156351	4.659752
C	1.651022	-0.165263	4.171536
C	-1.955860	-1.873071	2.934464
C	-2.803937	-2.322299	3.923050
C	-2.446325	-2.204165	5.296306
O	-4.006880	-2.887756	3.696812
N	0.812199	-0.600161	5.082859
C	-4.409264	-3.044175	2.345180
C	-0.017545	-0.980540	0.848181
C	0.727588	-2.190055	0.243369
C	-1.078094	-3.741960	-0.484344
C	1.053157	-3.374663	1.164188
C	1.084841	-4.644403	0.293286
C	-0.370125	-5.039352	-0.046678
C	0.242455	-0.815314	2.332990
N	-0.056721	-2.735360	-0.928910
C	-1.259625	-1.632891	5.649601
N	0.444150	0.212276	0.120111
C	-0.251306	1.258517	-0.148816
C	-1.654638	1.495061	0.302342
C	-1.647211	2.709215	1.256834
C	-1.017073	3.947894	0.601939
C	0.402496	3.625033	0.113783
C	0.418477	2.409529	-0.833583
C	-1.034708	5.140965	1.535952
C	-1.750135	6.292356	1.202027
C	-1.774694	7.392546	2.056389
C	-1.080166	7.354839	3.261664
C	-0.362183	6.211124	3.606351
C	-0.340496	5.114405	2.750523
H	1.987390	-5.252763	-1.593553
H	2.768065	-3.852692	-0.844433
H	0.325389	-3.908322	-2.623347
H	1.500616	-2.592268	-2.334835
H	-2.235260	-7.290434	1.870818
H	-1.685687	-7.460667	0.110411
H	-1.164633	-5.108865	2.021887
H	2.164991	0.113405	2.082403
H	2.577689	0.277005	4.531479
H	-2.265519	-1.928251	1.896709
H	-3.147146	-2.573617	6.037986
H	-5.405287	-3.486270	2.378994
H	-4.444491	-2.082728	1.822271
H	-3.728852	-3.718189	1.808104
H	-1.086262	-1.093470	0.653763
H	1.663142	-1.830733	-0.197568
H	-1.769392	-3.892287	-1.316584
H	-1.642737	-3.285907	0.330747
H	0.315642	-3.475751	1.967639
H	2.022264	-3.193293	1.636755
H	1.584006	-5.459739	0.822180
H	-0.350237	-5.747884	-0.884083
H	-0.967802	-1.524622	6.689359
H	-2.247021	1.739121	-0.588618
H	-2.105964	0.623164	0.778459
H	-1.091416	2.447804	2.166080
H	-2.676572	2.921569	1.560158
H	-1.623009	4.203228	-0.279121
H	1.050126	3.410624	0.973413
H	0.832816	4.487100	-0.404278
H	1.439984	2.147086	-1.118422
H	-0.154602	2.640391	-1.740125
H	-2.295196	6.326812	0.261541
H	-2.337949	8.278475	1.778443
H	-1.096777	8.210994	3.929120
H	0.183338	6.172961	4.544596
H	0.224296	4.229048	3.034624
C	-2.798380	-0.903881	-1.344771
O	-1.668662	-0.824983	-1.908520
O	-3.064391	-1.447441	-0.254761
C	-3.945698	-0.228965	-2.085292
C	-3.718723	0.383623	-3.316016
C	-5.222637	-0.219973	-1.529768
C	-4.781847	0.993504	-3.968435
H	-2.725241	0.375280	-3.749043
C	-6.251478	0.404073	-2.221731
H	-5.401081	-0.696975	-0.573424
C	-6.066499	1.023591	-3.448356
H	-6.882352	1.505723	-3.971515
N	-7.601181	0.414723	-1.633498
O	-7.749790	-0.136534	-0.559273
O	-8.482462	0.974971	-2.257879
N	-4.542475	1.639721	-5.269635
O	-5.494507	2.152141	-5.827574
O	-3.406334	1.621110	-5.704301
C	3.705970	-0.337309	-0.894920
O	3.020223	0.480821	-0.204507
O	3.310702	-1.382781	-1.431175
C	5.174026	0.024026	-1.058576
C	6.007260	-0.815663	-1.793596
C	5.689976	1.178060	-0.474935
C	7.346278	-0.478928	-1.932681
H	5.603465	-1.715088	-2.243304
C	7.036972	1.469923	-0.642864
H	5.045467	1.831012	0.101084
C	7.897782	0.661474	-1.368759
H	8.945490	0.906361	-1.487771
N	7.583857	2.687778	-0.022941
O	8.761338	2.933558	-0.207860
O	6.824719	3.372842	0.636473
N	8.228616	-1.366943	-2.707332
O	7.733734	-2.365765	-3.194511
O	9.398172	-1.047115	-2.811468
H	-0.599228	-1.940306	-1.392179
H	1.501528	0.242974	-0.124349

Oxindole

E_{313}: -439.028327
qh-G_{313}: -438.919773

C	-1.305047	-1.425673	-0.000054
C	-0.150851	-0.657455	-0.000023
C	-0.188621	0.744788	0.000021
C	-1.408676	1.396802	0.000033
C	-2.586047	0.639847	0.000002
C	-2.528745	-0.751350	-0.000042
H	-1.259860	-2.510134	-0.000088
H	-1.452770	2.482442	0.000067
H	-3.548575	1.141089	0.000011
H	-3.448939	-1.327712	-0.000065
C	1.227074	1.254631	0.000046
H	1.479324	1.851333	-0.882707
H	1.479312	1.851283	0.882836
N	1.181398	-1.079875	-0.000027
C	2.069919	-0.024661	0.000015
O	3.277428	-0.118373	0.000024
H	1.488270	-2.043778	-0.000050

TS1, path to (a*R*)-product

E_{313}: -3579.620898
qh-G_{313}: -3578.678836
im. freq: -242.66 cm^{-1}

C	1.789389	2.199912	-1.838221
C	2.070521	3.429423	-2.509058
N	1.120883	4.192998	-3.118463
C	-0.116262	3.761944	-3.091053
C	-0.510055	2.557861	-2.461249
C	0.424951	1.771182	-1.833710
C	2.854603	1.491407	-1.227200
C	4.147521	1.971698	-1.302740
C	4.429254	3.182801	-1.986849
C	3.408272	3.890132	-2.563089
O	5.107135	1.238131	-0.685771

C	6.446308	1.697900	-0.747728
C	-0.026892	0.444640	-1.223859
C	-0.341763	-0.485666	-2.413167
N	-0.644271	-1.898688	-1.988034
C	0.771415	-0.561068	-3.477995
C	0.781990	-1.967976	-4.096596
C	0.622152	-2.659795	-1.722522
C	1.333292	-2.969181	-3.058929
C	2.825152	-2.883602	-2.886872
C	3.643444	-3.930998	-2.877856
C	-0.661812	-2.374311	-4.417998
C	-1.419620	-2.565032	-3.091951
H	-0.864351	4.380904	-3.583257
H	-1.558068	2.268765	-2.475279
H	2.687704	0.571341	-0.670851
H	5.444001	3.556423	-2.052759
H	3.595569	4.823789	-3.083655
H	7.036634	0.989557	-0.163339
H	6.816781	1.715959	-1.779488
H	6.549710	2.691723	-0.298325
H	0.765488	0.012453	-0.608755
H	-1.275493	-0.128647	-2.861378
H	1.745059	-0.332482	-3.031331
H	0.587539	0.199899	-4.240771
H	1.400327	-1.979683	-4.997509
H	0.356206	-3.556932	-1.161231
H	1.256626	-2.040009	-1.089137
H	1.078782	-3.985943	-3.382607
H	3.247515	-1.885355	-2.757266
H	4.714927	-3.806030	-2.751322
H	3.274988	-4.946976	-3.003561
H	-0.682665	-3.305148	-4.991091
H	-1.143680	-1.602092	-5.026410
H	-1.519056	-3.613717	-2.803832
H	-2.407523	-2.103467	-3.098274
H	-1.284043	-1.899713	-1.151871
N	-1.243789	0.611968	-0.430917
C	-1.375251	1.053313	0.836590
C	-2.673136	1.795457	1.092609
C	-0.174663	1.635969	1.545101
C	-2.485377	3.274726	0.721771
H	-2.933782	1.732832	2.151600
H	-3.480854	1.340686	0.507132
C	-0.035132	3.142486	1.258192
H	-0.325216	1.511042	2.622799
H	0.745649	1.101378	1.281936
C	-1.341961	3.900126	1.536485
H	-3.420961	3.812523	0.908611
H	-2.263874	3.371890	-0.349375
H	0.771561	3.540741	1.882427
H	0.259307	3.305667	0.216921
H	-1.587192	3.774686	2.601618
H	-2.118523	0.392297	-0.933126
C	3.078723	-1.718317	1.717412
O	2.299855	-1.357395	0.766362
O	2.750373	-1.972472	2.880878
C	-3.781312	-1.345228	-1.040215
O	-2.944509	-2.131341	-0.534698
O	-3.539134	-0.330937	-1.744205
C	-0.470578	-0.247312	5.397579
C	-0.747339	-0.543168	4.069156
C	-2.000674	-0.282697	3.470999
C	-3.014836	0.274235	4.254085
C	-2.754085	0.566269	5.590059
C	-1.497149	0.313761	6.152842
H	0.504080	-0.454086	5.828412
H	-3.997951	0.462162	3.830754
H	-3.538636	0.992602	6.207511
H	-1.319142	0.551667	7.196862
C	-1.894750	-0.649775	2.066882
H	-2.712399	-0.940080	1.421538
C	-0.622165	-1.256835	1.951885
N	0.073529	-1.123920	3.102749
H	1.051139	-1.437008	3.208752
O	-0.102921	-1.787090	0.881622
H	0.961911	-1.683633	0.911791
C	-5.245979	-1.647549	-0.761446
C	-5.594383	-2.774709	-0.020436
C	-6.237933	-0.802343	-1.252240
C	-6.938062	-3.034490	0.211777
H	-4.822168	-3.431734	0.362363
C	-7.567151	-1.105377	-0.989300
H	-5.965134	0.071896	-1.831381
C	-7.954967	-2.218346	-0.259047
H	-8.997064	-2.438727	-0.066329
N	-7.308923	-4.229141	0.988664
O	-6.406962	-4.934762	1.398270
O	-8.494295	-4.436509	1.170981
N	-8.617469	-0.212924	-1.506381
O	-8.263705	0.763338	-2.140387
O	-9.774067	-0.506657	-1.267563
C	4.536192	-1.830805	1.337457
C	5.485709	-2.166719	2.298831
C	4.926033	-1.590807	0.024737
C	6.819328	-2.244129	1.920264
H	5.181673	-2.359840	3.321313
C	6.272128	-1.664623	-0.298606
H	4.191617	-1.329058	-0.725271
C	7.251788	-1.987671	0.627088
H	8.299919	-2.032955	0.359145
N	6.679176	-1.331280	-1.669880
O	5.801817	-1.194304	-2.503661
O	7.869708	-1.197289	-1.887211
N	7.828581	-2.598180	2.931433
O	8.990214	-2.649516	2.571146
O	7.438486	-2.816130	4.062215
C	-1.201421	5.382512	1.260078
C	-1.483706	6.325528	2.250189
C	-0.795732	5.839822	0.001535
C	-1.362692	7.689956	1.994609
H	-1.800561	5.986002	3.233641
C	-0.671755	7.200757	-0.258288
H	-0.569519	5.123919	-0.785781
C	-0.955477	8.131887	0.739080
H	-1.584278	8.407479	2.779420
H	-0.349413	7.532970	-1.240944
H	-0.857708	9.194645	0.538523

GS3, path to (a*R*)-product

E_{313}: -3579.635699
qh-G_{313}: -3578.691377

C	-0.131826	4.012388	0.130526
C	0.100049	5.367205	-0.245264
N	1.269612	6.019824	-0.014874
C	2.229405	5.352306	0.587499
C	2.110653	4.006673	0.990662
C	0.937311	3.322009	0.770444
C	-1.387277	3.411561	-0.176658
C	-2.356537	4.136161	-0.830685
C	-2.130181	5.493601	-1.191803
C	-0.936270	6.086718	-0.906913
O	-3.568624	3.650008	-1.185957
C	-3.824746	2.293964	-0.879804
C	0.850933	1.851176	1.190439
C	0.908895	1.828374	2.727052
N	0.626977	0.467058	3.308981
C	-0.075444	2.807143	3.403347
C	-0.565102	2.193990	4.721649
C	-0.837510	0.162471	3.317350
C	-1.524220	1.026286	4.392226
C	-2.897085	1.510996	4.006932
C	-3.618733	1.140571	2.952008
C	0.639252	1.629156	5.486544
C	1.170176	0.414198	4.706622
H	3.162232	5.886612	0.758985
H	2.964418	3.500876	1.434132
H	-1.568943	2.377042	0.087779
H	-2.927658	6.025436	-1.700657
H	-0.734869	7.118515	-1.176981
H	-4.824856	2.079578	-1.260347
H	-3.094132	1.637549	-1.369380
H	-3.797907	2.122374	0.203472
H	-0.111728	1.439863	0.881282
H	1.940826	2.048674	3.026988

H	-0.932322	2.999020	2.744946
H	0.424022	3.764277	3.572362
H	-1.084852	2.947159	5.320605
H	-0.937236	-0.909919	3.500457
H	-1.205971	0.371896	2.311309
H	-1.638700	0.430994	5.309915
H	-3.326170	2.227662	4.707725
H	-4.613521	1.549676	2.796771
H	-3.278735	0.408596	2.224253
H	0.350019	1.322145	6.495543
H	1.414458	2.395752	5.585752
H	0.832961	-0.536191	5.126031
H	2.257223	0.383801	4.610213
H	1.116960	-0.339037	2.812154
N	1.947533	1.082964	0.631758
C	1.884890	0.331112	-0.616839
C	3.355184	0.042964	-0.985713
C	1.243970	1.139394	-1.762196
C	4.133124	1.310667	-1.332490
H	3.383567	-0.613901	-1.859063
H	3.836162	-0.489334	-0.152428
C	2.051099	2.356700	-2.219939
H	1.122618	0.446593	-2.608508
H	0.233605	1.459785	-1.476357
C	3.502575	2.009049	-2.548986
H	5.175219	1.049104	-1.549022
H	4.138364	2.003263	-0.482989
H	1.557561	2.807838	-3.089213
H	2.043772	3.106799	-1.426272
H	3.504202	1.282657	-3.376905
H	2.548470	0.639183	1.325125
C	-4.306168	-1.237502	-0.953758
O	-3.756559	-0.566379	0.036196
O	-3.695629	-1.757400	-1.869320
C	2.958266	-1.597668	2.441978
O	1.723817	-1.823867	2.615561
O	3.549437	-0.520922	2.649092
C	0.216692	-3.678315	-2.928023
C	0.267362	-2.607210	-2.050771
C	1.435020	-2.201690	-1.395680
C	2.596299	-2.936518	-1.604885
C	2.573416	-4.026995	-2.479017
C	1.399235	-4.387765	-3.137277
H	-0.710448	-3.963335	-3.414794
H	3.517327	-2.678435	-1.090886
H	3.480384	-4.602287	-2.640118
H	1.398003	-5.239290	-3.810143
C	1.100448	-1.051116	-0.461554
C	-0.409660	-0.930613	-0.667050
N	-0.796899	-1.800266	-1.617625
H	-1.776078	-1.898621	-1.894135
O	-1.194079	-0.174654	-0.062430
H	-2.752470	-0.471908	-0.085982
C	3.754814	-2.741723	1.837494
C	3.103855	-3.909857	1.447796
C	5.116302	-2.584629	1.586464
C	3.828368	-4.893545	0.788990
H	2.041326	-4.024652	1.627077
C	5.799838	-3.607273	0.941809
H	5.620123	-1.670577	1.880575
C	5.182187	-4.774813	0.517102
H	5.728622	-5.549492	-0.005468
N	3.120764	-6.086537	0.296702
O	1.939522	-6.190036	0.564152
O	3.761880	-6.891485	-0.354315
N	7.238759	-3.446304	0.674444
O	7.771982	-2.426698	1.068126
O	7.803548	-4.343663	0.076698
C	-5.797941	-1.308139	-0.855701
C	-6.492046	-2.061172	-1.800369
C	-6.481393	-0.630268	0.151973
C	-7.873998	-2.122533	-1.709877
H	-5.961285	-2.585994	-2.586633
C	-7.864530	-0.724353	0.191450
H	-5.950140	-0.043130	0.891555
C	-8.594611	-1.464585	-0.724677
H	-9.674511	-1.526987	-0.673426
N	-8.592392	-0.006548	1.252568
O	-7.934263	0.661101	2.027535
O	-9.801111	-0.128596	1.282046
N	-8.616462	-2.918282	-2.703625
O	-9.828087	-2.941426	-2.607459
O	-7.967367	-3.497389	-3.552348
C	4.341316	3.196014	-2.986673
C	5.532595	2.956971	-3.682510
C	4.004091	4.520284	-2.694317
C	6.365052	4.000672	-4.070481
H	5.805337	1.931268	-3.924383
C	4.836548	5.570730	-3.080890
H	3.082039	4.750677	-2.168608
C	6.018934	5.316844	-3.767827
H	7.282029	3.787871	-4.612579
H	4.552536	6.592124	-2.843401
H	6.664122	6.136591	-4.069606
H	1.245770	-1.380685	0.576014

TS2, path to (a*R*)-product

E_{313}: -3579.621844
qh-G_{313}: -3580.064097
im. freq: -240.53 cm^{-1}

C	-0.084053	3.654417	1.812490
C	0.583920	4.756198	2.424937
N	1.830952	4.676547	2.959872
C	2.444355	3.518517	2.911860
C	1.885539	2.364410	2.319726
C	0.635116	2.423895	1.746309
C	-1.397303	3.837130	1.301318
C	-2.004577	5.071143	1.382115
C	-1.329756	6.173998	1.975390
C	-0.074689	6.015821	2.484029
O	-3.243943	5.344225	0.927684
C	-3.997952	4.250881	0.435871
C	0.084785	1.171326	1.076400
C	-0.139622	0.124329	2.194139
N	-0.364154	-1.260273	1.660461
C	-1.347197	0.505071	3.081689
C	-2.261562	-0.714389	3.244945
C	-1.646273	-1.361491	0.902773
C	-2.831314	-1.126334	1.863179
C	-3.863672	-0.139970	1.376771
C	-3.801222	0.678946	0.327812
C	-1.443224	-1.882884	3.806449
C	-0.344462	-2.246291	2.789045
H	3.438555	3.468451	3.350889
H	2.463817	1.441298	2.312730
H	-1.916681	3.009394	0.834369
H	-1.848243	7.126642	2.013651
H	0.458441	6.837307	2.951508
H	-4.946046	4.664160	0.089670
H	-3.489058	3.762277	-0.401333
H	-4.179562	3.522115	1.236521
H	-0.869307	1.376422	0.579919
H	0.782778	0.038631	2.771809
H	-1.907015	1.328535	2.624341
H	-0.994611	0.855100	4.055520
H	-3.086615	-0.471902	3.920957
H	-1.666777	-2.348179	0.437075
H	-1.600520	-0.635101	0.092914
H	-3.348848	-2.084259	2.011987
H	-4.764383	-0.120259	1.991915
H	-4.634213	1.332083	0.082328
H	-2.956764	0.715521	-0.356273
H	-2.087839	-2.747913	3.985681
H	-0.996447	-1.597766	4.763383
H	-0.496294	-3.227928	2.334847
H	0.662948	-2.211806	3.210210
H	0.458288	-1.556096	1.032570
N	1.005509	0.719036	0.021877
C	1.047875	1.748683	-1.681159
C	1.854545	0.745478	-2.492710
C	1.822149	2.995323	-1.324452
C	3.282460	0.511281	-2.004910
H	1.894359	1.190857	-3.497898
H	1.311648	-0.196225	-2.598237

C	3.258333	2.745362	-0.860497
H	1.835468	3.597108	-2.246510
H	1.273342	3.578550	-0.579981
C	4.047940	1.824705	-1.801192
H	3.807209	-0.117465	-2.732412
H	3.283403	-0.056758	-1.065835
H	3.771627	3.707603	-0.760823
H	3.249821	2.302245	0.141958
H	4.129799	2.321979	-2.778525
H	1.930225	0.530649	0.424667
C	-4.113909	-1.433431	-1.984538
O	-2.917329	-1.793451	-1.760005
O	-4.505448	-0.528386	-2.737346
C	2.743477	-1.775901	0.783613
O	1.676002	-2.172846	0.232050
O	2.844559	-0.840396	1.609358
C	-3.467752	3.469975	-3.040805
C	-2.421711	2.621547	-2.692532
C	-1.171684	3.079995	-2.205502
C	-1.009348	4.464134	-2.037333
C	-2.058597	5.318993	-2.359605
C	-3.271171	4.834658	-2.868740
H	-4.399914	3.068646	-3.427089
H	-0.087099	4.881955	-1.649715
H	-1.930951	6.387040	-2.212229
H	-4.066726	5.528828	-3.120681
C	-0.340648	1.894361	-2.027569
H	-1.780136	-1.055061	-2.157844
C	-1.170575	0.803057	-2.356417
N	-2.384760	1.236018	-2.761717
H	-3.192078	0.611012	-2.945168
O	-0.889364	-0.473636	-2.217456
C	4.015052	-2.485926	0.364405
C	4.002100	-3.357540	-0.722349
C	5.201097	-2.245501	1.053346
C	5.190775	-3.962234	-1.107150
H	3.077761	-3.551771	-1.254085
C	6.360066	-2.883098	0.633138
H	5.209678	-1.572537	1.903105
C	6.392654	-3.745415	-0.451458
H	7.308887	-4.225576	-0.770777
N	5.184436	-4.878037	-2.259713
O	4.128773	-5.039744	-2.841581
O	6.235149	-5.414729	-2.557348
N	7.612802	-2.634255	1.361483
O	7.550108	-1.968502	2.380074
O	8.634027	-3.112957	0.907366
C	-5.161480	-2.193351	-1.193372
C	-6.515370	-1.940825	-1.395841
C	-4.763599	-3.089355	-0.206139
C	-7.444858	-2.601521	-0.602657
H	-6.829048	-1.234829	-2.156331
C	-5.729282	-3.700080	0.580210
H	-3.711786	-3.298414	-0.054796
C	-7.087704	-3.486973	0.403059
H	-7.829770	-3.977475	1.020432
N	-5.292316	-4.588847	1.665798
O	-4.101489	-4.605862	1.933412
O	-6.140973	-5.242658	2.238831
N	-8.878140	-2.340241	-0.818656
O	-9.668865	-2.899161	-0.081380
O	-9.180182	-1.581571	-1.719547
C	5.447095	1.571245	-1.279472
C	6.570730	1.944584	-2.019070
C	5.639642	0.948676	-0.040268
C	7.856552	1.703120	-1.538949
H	6.436101	2.427118	-2.984424
C	6.922260	0.713868	0.446721
H	4.777554	0.634651	0.548780
C	8.036373	1.087385	-0.303664
H	8.717837	1.997495	-2.131488
H	7.056018	0.237493	1.414255
H	9.036424	0.900312	0.076041
H	0.694289	-0.166441	-0.390635

9-*epi*-NH_2-QDA · [3,5-DNBA]$_2$

E_{313}: -2676.137641

qh-G_{313}: -2675.52811

C	-1.745226	5.053654	0.399083
H	-2.247067	5.689887	-0.335676
C	-2.607771	3.812959	0.703064
H	-3.499235	3.734056	0.079415
C	1.164506	2.256176	-2.500509
H	1.290898	4.324122	-2.301456
H	2.130936	2.195462	-2.994228
H	-2.914900	3.757853	1.750116
C	0.689316	3.435276	-2.104796
C	1.076029	1.144808	3.512919
H	-1.600113	5.649529	1.305172
C	2.682994	1.150030	1.724535
C	3.686112	1.053380	2.734852
C	2.152888	1.062611	4.429847
C	3.089113	1.223965	0.371112
C	4.426592	1.196453	0.028651
C	5.421900	1.073382	1.031339
O	4.709537	1.277556	-1.297107
N	3.408905	1.009505	4.068958
C	6.070234	1.370799	-1.684230
C	0.145717	1.197150	1.191231
C	-0.598371	2.538487	1.305626
C	-1.467139	2.511971	-1.031006
H	0.235536	5.452805	-0.388171
C	0.308870	3.733820	0.923574
H	1.262320	3.365047	0.529502
H	0.535237	4.331508	1.810895
C	-0.388670	4.588947	-0.140399
C	-0.617328	3.741477	-1.415160
C	1.318299	1.174931	2.162575
N	-1.814084	2.573480	0.424134
H	1.946279	1.033889	5.497890
H	0.061652	1.171082	3.903334
C	5.047531	1.005928	2.349152
H	2.371174	1.317847	-0.437154
H	6.473014	1.039764	0.769262
H	5.787682	0.919737	3.138282
H	6.065652	1.498332	-2.767417
H	6.557811	2.235266	-1.219717
H	6.626790	0.460678	-1.426068
H	0.527935	1.110879	0.172812
H	-0.989231	2.642725	2.324342
N	-0.686922	0.002584	1.410769
H	-1.473403	-0.042989	0.758122
H	0.304808	-1.215124	1.127860
H	-2.423450	2.471239	-1.553743
H	-0.956498	1.561814	-1.201523
H	-1.204649	4.363385	-2.104381
H	0.644886	1.310937	-2.364885
C	3.470680	-1.432994	-1.846051
C	4.788088	-1.757936	-2.128427
C	5.560302	-2.557669	-1.300438
C	4.948814	-3.032222	-0.149650
C	3.639855	-2.722657	0.192834
C	2.901406	-1.917899	-0.672557
H	2.901882	-0.785946	-2.503539
H	6.590601	-2.793687	-1.535784
H	3.212597	-3.087524	1.119304
N	5.413892	-1.178918	-3.326139
O	6.587658	-1.432556	-3.527311
O	4.724699	-0.466527	-4.031111
N	5.738770	-3.877957	0.760522
O	5.175848	-4.323579	1.741551
O	6.904519	-4.075194	0.472646
C	1.518223	-1.451073	-0.325953
O	0.857055	-0.784657	-1.104949
O	1.142081	-1.784963	0.884476
C	-5.489910	-1.365818	0.737488
C	-6.521431	-2.291305	0.642672
C	-7.568232	-2.162487	-0.256678
C	-7.546760	-1.042603	-1.074353
C	-6.542616	-0.087326	-1.015696
C	-5.505004	-0.255250	-0.101852
H	-4.686126	-1.499644	1.451299
H	-8.361478	-2.896440	-0.319449
H	-6.551181	0.781585	-1.662995

N	-6.508931	-3.461747	1.534925
O	-7.413507	-4.267569	1.420691
O	-5.594889	-3.550250	2.333475
N	-8.643331	-0.868394	-2.040704
O	-8.615490	0.119055	-2.750289
O	-9.509933	-1.722739	-2.069282
C	-4.404950	0.790359	-0.038529
O	-3.461251	0.549673	0.784894
O	-4.508995	1.778690	-0.775978
H	-2.477832	1.736327	0.630021
H	-1.103641	0.004280	2.342024

(a*R*)-product

E_{313}: -903.476132
qh-G_{313}: -903.168617

C	-3.842486	-2.619977	0.275795
C	-5.000240	-2.112105	-0.306979
C	-5.072863	-0.774022	-0.695094
C	-3.966584	0.026512	-0.460369
C	-2.794382	-0.447186	0.166104
C	-2.736489	-1.797550	0.505117
N	-3.792983	1.362257	-0.804774
C	-2.531664	1.826112	-0.493947
C	-1.843625	0.686707	0.223779
C	-0.648466	0.808127	0.843676
O	-2.143246	2.951024	-0.751828
C	-0.027140	-0.264929	1.695248
C	1.259140	-0.782457	1.029794
C	2.249579	0.369760	0.798116
C	1.575330	1.504786	0.011241
C	0.274347	1.988258	0.683344
C	3.525572	-0.098405	0.129817
C	4.761238	0.068999	0.758652
C	5.940806	-0.350324	0.147301
C	5.901140	-0.947514	-1.108920
C	4.674701	-1.120647	-1.748230
C	3.499575	-0.699188	-1.133867
H	-3.790160	-3.669048	0.548582
H	-5.851295	-2.764144	-0.478712
H	-5.959696	-0.371430	-1.174514
H	-1.839906	-2.239374	0.922441
H	-4.462764	1.930491	-1.305339
H	-0.715970	-1.076849	1.920459
H	0.244988	0.194936	2.656227
H	1.005534	-1.251742	0.070181
H	1.721930	-1.553419	1.655572
H	2.519226	0.770752	1.786248
H	1.342484	1.156691	-1.003655
H	2.268900	2.346463	-0.091231
H	-0.182772	2.787721	0.104989
H	0.520309	2.377736	1.681413
H	4.799331	0.535311	1.740568
H	6.891285	-0.209576	0.653900
H	6.818528	-1.275893	-1.588342
H	4.632764	-1.584727	-2.729467
H	2.549203	-0.837641	-1.644752

TS1, path to (a*S*)-product

E_{313}: -3579.61743
qh-G_{313}: -3578.676956
im. freq: -154.25 cm^{-1}

C	4.741663	-0.981105	-1.855289
C	5.100616	-0.677442	-3.200804
N	4.203831	-0.309778	-4.151920
C	2.938684	-0.235359	-3.805844
C	2.470807	-0.488430	-2.498606
C	3.364130	-0.849937	-1.515690
C	5.757866	-1.382759	-0.940386
C	7.066734	-1.470487	-1.357162
C	7.426620	-1.142193	-2.694371
C	6.469436	-0.760098	-3.585770
O	8.098229	-1.867435	-0.579326
C	7.787835	-2.356006	0.710564
C	2.835520	-1.064052	-0.102423
C	2.116980	-2.416675	-0.027398
N	1.551859	-2.645315	1.352007
C	2.999479	-3.629781	-0.372647
C	2.571808	-4.804824	0.519247
C	2.606826	-3.082550	2.313918
C	3.038695	-4.519668	1.967152
C	4.510939	-4.773589	2.163146
C	5.396971	-3.983874	2.767990
C	1.038676	-4.901849	0.517016
C	0.471538	-3.685378	1.270039
H	2.233596	0.050588	-4.583886
H	1.412856	-0.370539	-2.270316
H	5.499490	-1.641589	0.079706
H	8.472655	-1.218048	-2.972955
H	6.714350	-0.515471	-4.614311
H	8.730040	-2.693997	1.143277
H	7.359867	-1.569456	1.345194
H	7.086767	-3.196961	0.649085
H	3.663982	-1.049108	0.611679
H	1.233610	-2.371031	-0.676394
H	4.060656	-3.406626	-0.207708
H	2.878106	-3.872057	-1.431759
H	3.018493	-5.736327	0.160740
H	2.193640	-2.984368	3.320362
H	3.436838	-2.379430	2.216342
H	2.503424	-5.219841	2.624528
H	4.849952	-5.738045	1.783866
H	6.430509	-4.298455	2.881040
H	5.141146	-3.022702	3.207879
H	0.707328	-5.824701	1.000900
H	0.664482	-4.911698	-0.511571
H	0.188811	-3.915214	2.300320
H	-0.368679	-3.226715	0.746239
H	1.096493	-1.759133	1.730624
N	1.898740	-0.010114	0.262486
C	2.210586	1.130278	0.863920
C	1.144524	2.191810	0.815313
C	3.618650	1.666299	0.839568
C	1.327875	2.978099	-0.494863
H	1.267674	2.869843	1.667054
H	0.148641	1.740133	0.857099
C	3.802008	2.489517	-0.453687
H	3.754181	2.323402	1.704061
H	4.371958	0.874249	0.894123
C	2.735747	3.588091	-0.581917
H	0.571391	3.767341	-0.551424
H	1.156685	2.304066	-1.345139
H	4.802935	2.933955	-0.449375
H	3.748935	1.826146	-1.325310
H	2.852286	4.268185	0.274627
H	0.892605	-0.137620	-0.021095
C	-2.933807	0.260749	1.979279
O	-2.267571	-0.861851	1.872012
O	-2.482380	1.312857	2.398315
C	-1.233577	-1.057831	-1.066661
O	-0.775244	-2.209573	-1.190099
O	-0.649958	-0.031248	-0.623648
C	0.803196	3.449357	4.842643
C	1.042472	2.256184	4.173424
C	2.351410	1.785372	3.902659
C	3.441930	2.540146	4.345914
C	3.210568	3.733174	5.026293
C	1.908281	4.185391	5.266618
H	-0.209775	3.792622	5.029838
H	4.458055	2.197649	4.166121
H	4.053591	4.322497	5.374216
H	1.752997	5.122196	5.792550
C	2.210263	0.578095	3.122206
H	2.980150	-0.166295	2.959794
C	0.821804	0.296493	3.066790
N	0.143801	1.328550	3.663231
H	-0.852920	1.467740	3.508956
O	0.218463	-0.679567	2.499716
H	-1.290155	-0.713650	2.129631
C	-2.678033	-0.849485	-1.509836
C	-3.431635	-1.941137	-1.935477
C	-3.254784	0.417724	-1.466508
C	-4.755799	-1.744243	-2.300813
H	-2.982232	-2.927084	-1.964382

C	-4.585453	0.562634	-1.838470
H	-2.671383	1.265248	-1.122507
C	-5.369180	-0.501159	-2.261955
H	-6.410137	-0.370985	-2.532429
N	-5.566906	-2.903867	-2.706735
O	-4.986523	-3.949783	-2.917951
O	-6.769415	-2.736123	-2.801943
N	-5.222736	1.880492	-1.699018
O	-4.526963	2.811202	-1.342712
O	-6.422412	1.952624	-1.910203
C	-4.363425	0.149990	1.537685
C	-5.124320	1.316528	1.464848
C	-4.905365	-1.074166	1.152618
C	-6.434160	1.227241	1.017760
H	-4.690509	2.273405	1.733776
C	-6.222715	-1.103652	0.716778
H	-4.310643	-1.979655	1.172090
C	-7.018628	0.028866	0.637975
H	-8.036585	-0.013669	0.270053
N	-6.782994	-2.380474	0.243349
O	-6.004431	-3.306328	0.090292
O	-7.976382	-2.425793	0.029089
N	-7.226382	2.463311	0.882028
O	-8.397324	2.345175	0.579110
O	-6.653683	3.514590	1.087850
C	2.921696	4.399526	-1.847107
C	3.132371	5.778113	-1.783939
C	2.881309	3.788366	-3.105078
C	3.299990	6.531343	-2.943884
H	3.165768	6.267080	-0.812989
C	3.049468	4.536238	-4.266117
H	2.718727	2.714578	-3.178906
C	3.259861	5.911884	-4.189282
H	3.462534	7.602917	-2.872381
H	3.016605	4.043134	-5.233369
H	3.390764	6.495242	-5.095835

GS3, path to (a*S*)-product

E_{313}: -3579.628968
qh-G_{313}: -3578.684061

C	1.673919	-4.341753	-1.415631
C	2.839274	-5.146704	-1.563595
N	4.102268	-4.644005	-1.575471
C	4.239485	-3.343761	-1.455955
C	3.158203	-2.450408	-1.293117
C	1.871950	-2.937271	-1.244660
C	0.394144	-4.969726	-1.448171
C	0.293015	-6.332466	-1.612012
C	1.459658	-7.135586	-1.739247
C	2.693018	-6.554655	-1.716875
O	-0.871910	-7.019124	-1.671141
C	-2.071998	-6.281134	-1.572013
C	0.716250	-1.964929	-1.032173
C	0.643758	-1.025514	-2.243356
N	-0.588870	-0.154482	-2.098500
C	0.589280	-1.666140	-3.634587
C	-0.268220	-0.757383	-4.532589
C	-1.821412	-0.843305	-2.602085
C	-1.749038	-0.947981	-4.134493
C	-2.335091	-2.225753	-4.676554
C	-3.063687	-3.124756	-4.018531
C	0.105020	0.713735	-4.280530
C	-0.359690	1.113380	-2.866264
H	5.256061	-2.956027	-1.480635
H	3.346188	-1.382820	-1.186831
H	-0.504058	-4.370251	-1.374361
H	1.331082	-8.206315	-1.860799
H	3.600139	-7.141748	-1.820272
H	-2.882248	-7.005865	-1.657136
H	-2.145483	-5.768041	-0.604430
H	-2.153272	-5.546111	-2.383075
H	-0.221005	-2.526013	-0.994492
H	1.484580	-0.322961	-2.189106
H	0.158827	-2.675907	-3.593390
H	1.607910	-1.756731	-4.019646
H	-0.127163	-1.013553	-5.586228
H	-2.684493	-0.274960	-2.250501
H	-1.845064	-1.822665	-2.124167
H	-2.316095	-0.117267	-4.578874
H	-2.141446	-2.387939	-5.737146
H	-3.453579	-4.001666	-4.526800
H	-3.330951	-3.021352	-2.969507
H	-0.373379	1.361938	-5.020079
H	1.187437	0.853856	-4.346892
H	-1.303084	1.665296	-2.859317
H	0.413606	1.678688	-2.344528
H	-0.687728	0.005508	-1.079660
N	0.762243	-1.094087	0.140601
C	0.614480	-1.620470	1.505782
C	0.514467	-0.402028	2.448489
C	1.798554	-2.493746	1.971017
C	1.829601	0.374178	2.577752
H	0.214108	-0.761512	3.442109
H	-0.274089	0.267922	2.084369
C	3.107769	-1.703862	2.033737
H	1.583735	-2.861274	2.980138
H	1.900592	-3.370516	1.320572
C	2.988661	-0.535049	3.020001
H	1.698976	1.187235	3.301367
H	2.097678	0.837032	1.619365
H	3.925752	-2.370580	2.329142
H	3.357610	-1.312052	1.042161
H	2.728165	-0.952137	4.005196
H	1.575481	-0.474252	0.066943
C	-4.982726	0.871807	0.777595
O	-4.067979	0.802938	-0.165877
O	-4.964492	0.228388	1.811282
C	3.133217	1.547732	-1.465572
O	2.764475	1.475286	-2.651884
O	2.911091	0.731210	-0.530212
C	-2.881361	-2.703531	4.570538
C	-2.268402	-2.403369	3.366445
C	-1.091075	-3.022605	2.929422
C	-0.535627	-4.025967	3.710828
C	-1.135994	-4.349082	4.932104
C	-2.285100	-3.688641	5.359658
H	-3.790996	-2.199390	4.880502
H	0.346108	-4.566564	3.381751
H	-0.701263	-5.127848	5.550102
H	-2.735226	-3.950318	6.312158
C	-0.718283	-2.446450	1.578336
H	-0.672224	-3.242752	0.824899
C	-1.913113	-1.536125	1.290737
N	-2.705834	-1.506081	2.377913
H	-3.563107	-0.950403	2.401759
O	-2.129953	-0.899124	0.248394
H	-3.354164	0.133843	0.086731
C	3.970258	2.763470	-1.071852
C	4.613112	3.523175	-2.045932
C	4.113853	3.100486	0.271278
C	5.425374	4.578176	-1.648827
H	4.480639	3.280096	-3.093960
C	4.933246	4.165339	0.617725
H	3.612645	2.522714	1.038447
C	5.620547	4.921286	-0.318311
H	6.268607	5.738445	-0.028642
N	6.115615	5.371948	-2.677003
O	5.940963	5.061744	-3.840733
O	6.819069	6.293006	-2.302798
N	5.098268	4.488364	2.041954
O	4.277152	4.041228	2.818103
O	6.047524	5.187116	2.352534
C	-6.085701	1.834557	0.470609
C	-7.102728	1.989447	1.410485
C	-6.106016	2.557355	-0.720077
C	-8.131236	2.876126	1.133638
H	-7.086132	1.425959	2.336274
C	-7.159413	3.432022	-0.943930
H	-5.322040	2.444763	-1.458931
C	-8.191098	3.616600	-0.037166
H	-9.003607	4.305338	-0.233330
N	-7.187677	4.196194	-2.203071
O	-6.287553	3.997773	-2.996636
O	-8.107751	4.973035	-2.365817

N	-9.211835	3.040206	2.121772
O	-10.112993	3.806650	1.842517
O	-9.130187	2.396450	3.149645
C	4.268697	0.259124	3.185649
C	4.650407	0.708373	4.453730
C	5.067230	0.607814	2.090997
C	5.791149	1.485453	4.630638
H	4.038259	0.446389	5.314353
C	6.214969	1.379738	2.266437
H	4.769215	0.309008	1.088249
C	6.581521	1.823199	3.534664
H	6.063103	1.828228	5.624766
H	6.823432	1.639013	1.403393
H	7.470598	2.433009	3.666476

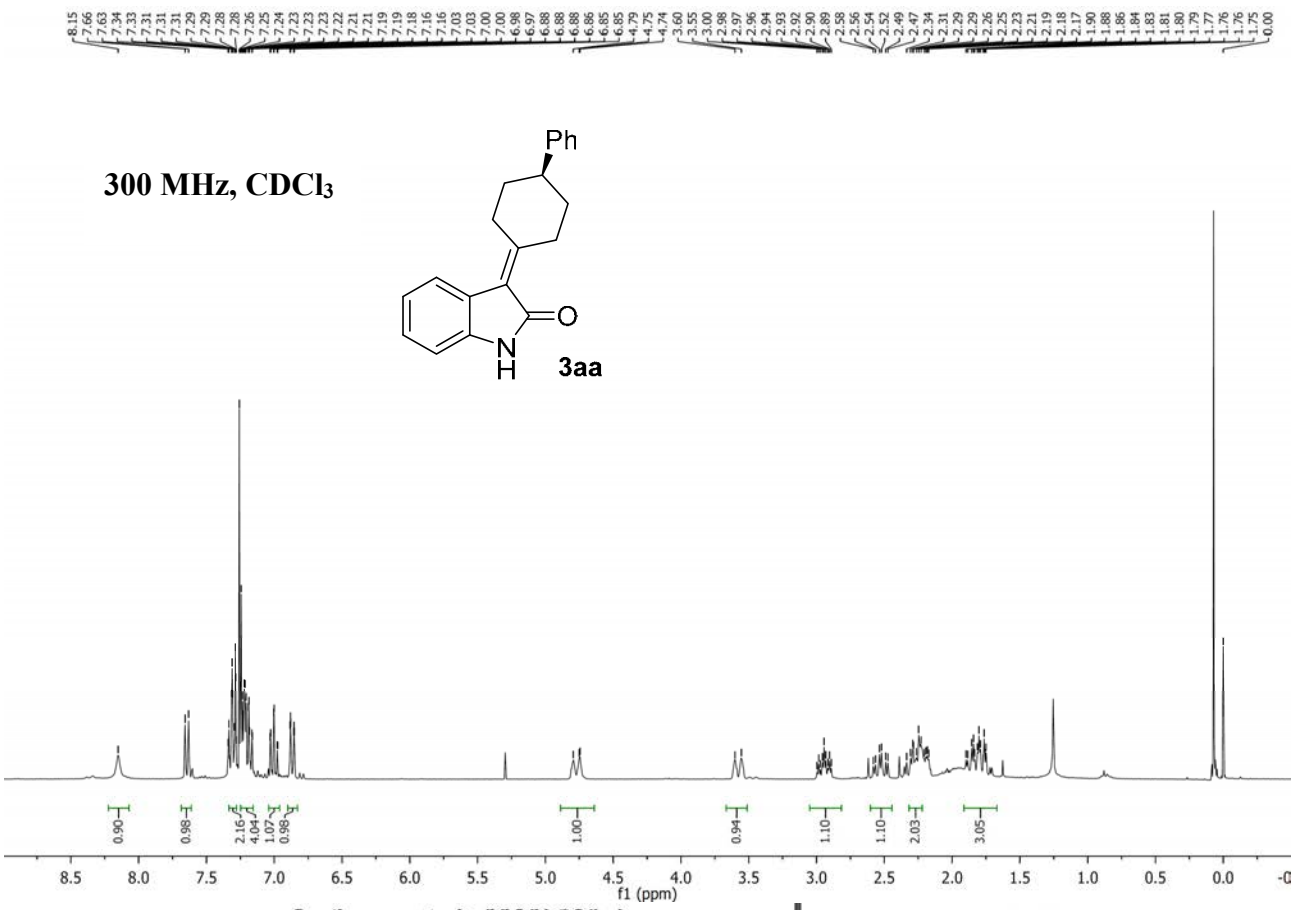
TS2, path to (a*S*)-product

E_{313}: -3579.613322
qh-G_{313}: -3578.670277
im. freq: -225.27 cm^{-1}

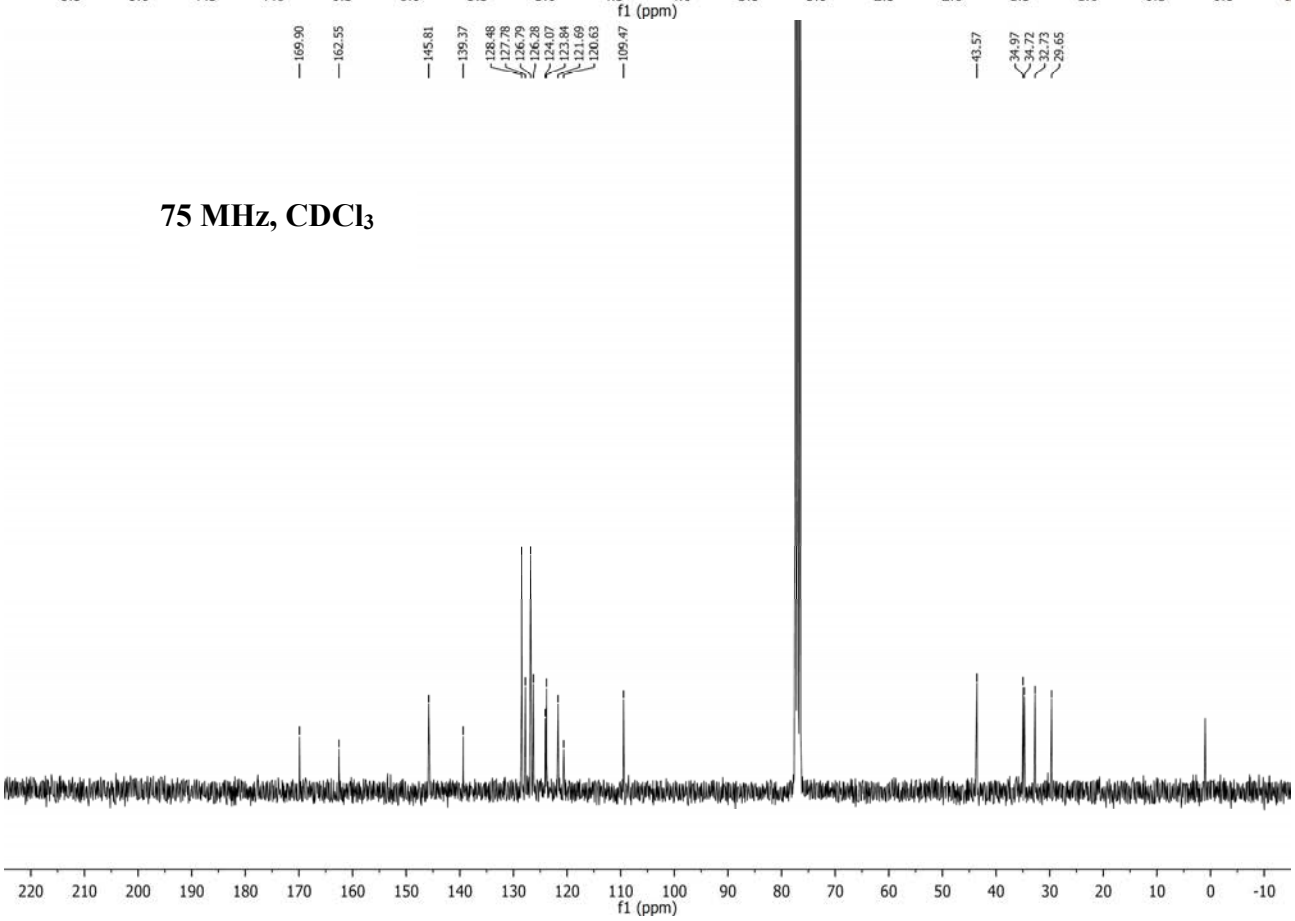
C	-0.287863	2.124886	2.581433
C	-0.090894	3.351541	3.281777
N	1.128900	3.818979	3.653303
C	2.178579	3.088124	3.361352
C	2.104175	1.858730	2.672014
C	0.881755	1.376718	2.254473
C	-1.613043	1.712149	2.267477
C	-2.686582	2.485558	2.648554
C	-2.486669	3.720450	3.326780
C	-1.225402	4.138503	3.629241
O	-3.979201	2.161493	2.434888
C	-4.238797	0.871240	1.907858
C	0.847762	0.061165	1.486276
C	1.199864	-1.061510	2.489375
N	1.432363	-2.396090	1.825619
C	0.095002	-1.261252	3.547839
C	-0.048558	-2.757238	3.853744
C	0.141541	-3.006432	1.376431
C	-0.651091	-3.469747	2.613611
C	-2.140187	-3.253080	2.510352
C	-2.787469	-2.358993	1.765104
C	1.343948	-3.344571	4.114153
C	2.137179	-3.301367	2.796468
H	3.146813	3.470279	3.678197
H	3.020894	1.301419	2.481443
H	-1.779646	0.794247	1.717988
H	-3.362797	4.301771	3.595100
H	-1.044142	5.072242	4.151636
H	-5.323205	0.797285	1.810473
H	-3.762311	0.739180	0.932247
H	-3.880253	0.097009	2.598541
H	-0.160060	-0.123778	1.089578
H	2.163136	-0.821761	2.943089
H	-0.862041	-0.868339	3.184345
H	0.352043	-0.700365	4.450508
H	-0.698734	-2.904972	4.720294
H	0.377547	-3.824101	0.690363
H	-0.385967	-2.240198	0.807644
H	-0.486105	-4.545939	2.749080
H	-2.727431	-3.900266	3.161210
H	-3.871240	-2.293997	1.789405
H	-2.293806	-1.666627	1.085440
H	1.269662	-4.376744	4.467272
H	1.855342	-2.765648	4.889478
H	2.201530	-4.276558	2.308362
H	3.144432	-2.895644	2.909840
H	2.123130	-2.306220	1.022750
N	1.726617	0.152321	0.319257
C	0.706522	0.519698	-1.469510
C	1.945303	0.450221	-2.344005
C	0.196430	1.915857	-1.184214
C	2.984630	1.551014	-2.126412
H	1.565502	0.518195	-3.374073
H	2.424509	-0.526652	-2.263260
C	1.280834	2.971479	-0.974759
H	-0.425731	2.194306	-2.047529
H	-0.491344	1.898089	-0.335549
C	2.351210	2.946165	-2.072238
H	3.720731	1.504274	-2.936314
H	3.544810	1.371778	-1.198895
H	0.807634	3.958452	-0.935890
H	1.760198	2.823518	0.001490
H	1.851982	3.123562	-3.036212
H	2.553422	0.708631	0.533973
C	-5.426593	-0.270795	-0.989574
O	-4.756504	0.738283	-1.467889
O	-4.938708	-1.277835	-0.492521
C	4.328051	-1.540670	0.633437
O	3.454330	-2.233668	0.022512
O	4.160754	-0.911618	1.693374
C	-1.421840	-3.978919	-1.842216
C	-1.245969	-2.608815	-1.718708
C	0.016981	-1.971087	-1.791982
C	1.136510	-2.787228	-1.988608
C	0.974179	-4.167558	-2.120116
C	-0.287735	-4.761095	-2.054309
H	-2.411392	-4.419167	-1.764673
H	2.142844	-2.389458	-2.003701
H	1.852862	-4.786228	-2.276340
H	-0.389631	-5.836538	-2.163169
C	-0.208993	-0.548730	-1.508208
H	-3.727572	0.628929	-1.286606
C	-1.628410	-0.416090	-1.258106
N	-2.203316	-1.646784	-1.435787
H	-3.183853	-1.809743	-1.212192
O	-2.308998	0.605041	-0.956747
C	5.694841	-1.464894	-0.024391
C	5.948244	-2.137741	-1.217199
C	6.696627	-0.703042	0.572164
C	7.208999	-2.033296	-1.789634
H	5.172200	-2.733167	-1.683692
C	7.939369	-0.631094	-0.040178
H	6.496448	-0.180716	1.500241
C	8.232024	-1.286285	-1.226646
H	9.208119	-1.215928	-1.689390
N	7.478697	-2.742896	-3.051098
O	6.568786	-3.385973	-3.539501
O	8.594312	-2.641563	-3.525906
N	8.997463	0.176902	0.588527
O	8.714106	0.776462	1.608383
O	10.087636	0.194890	0.048625
C	-6.916130	-0.106623	-1.085811
C	-7.725732	-1.112804	-0.564059
C	-7.482918	1.023692	-1.671906
C	-9.102095	-0.965030	-0.639168
H	-7.282252	-1.990705	-0.108722
C	-8.866550	1.115120	-1.727421
H	-6.861099	1.813710	-2.076321
C	-9.708454	0.138447	-1.219101
H	-10.785809	0.234205	-1.271286
N	-9.475414	2.303353	-2.350631
O	-8.723729	3.154548	-2.784099
O	-10.689922	2.353431	-2.390666
N	-9.961799	-2.019916	-0.075816
O	-11.164918	-1.871207	-0.169429
O	-9.411588	-2.968695	0.449451
C	3.393374	4.028197	-1.881074
C	3.596102	5.007123	-2.856056
C	4.182466	4.068970	-0.725642
C	4.559831	5.999350	-2.687006
H	2.990064	4.991564	-3.758952
C	5.147123	5.056355	-0.552392
H	4.041142	3.321705	0.052992
C	5.339646	6.026201	-1.534659
H	4.700342	6.751510	-3.457783
H	5.749785	5.069607	0.351042
H	6.092384	6.797063	-1.400570
H	2.084748	-0.758683	0.022034

NMR TRACES

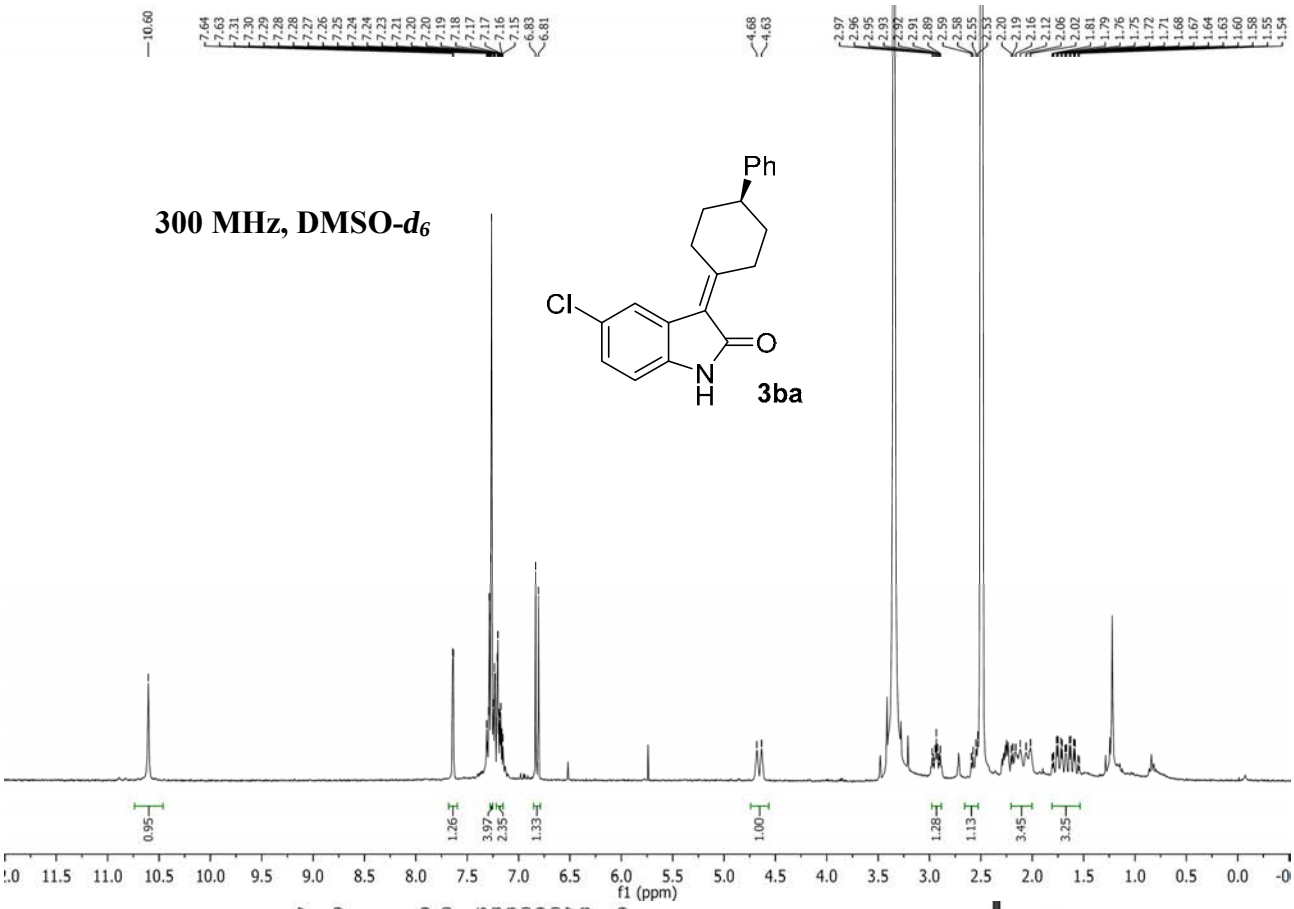
300 MHz, $CDCl_3$



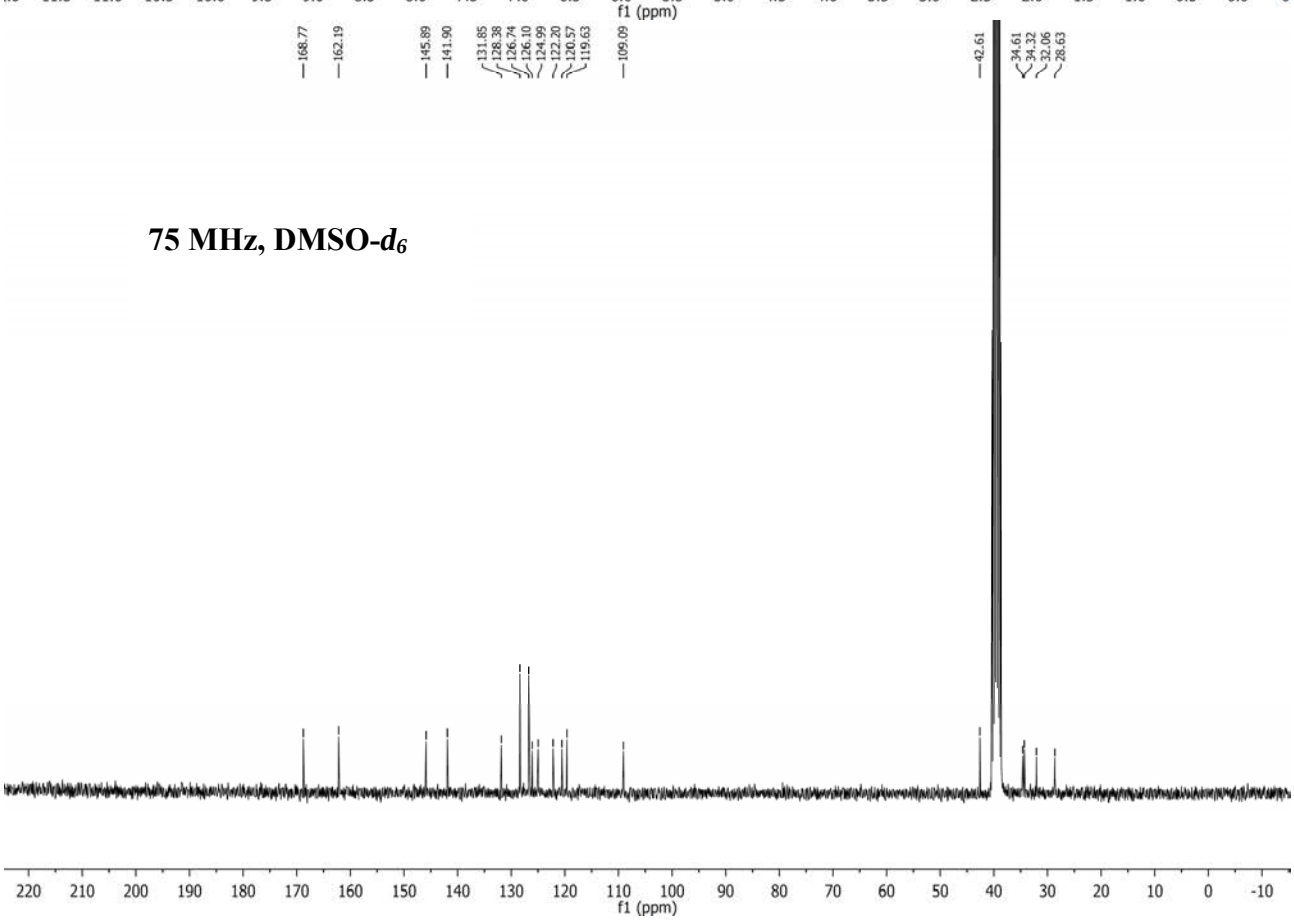
75 MHz, $CDCl_3$



300 MHz, DMSO-*d*$_6$

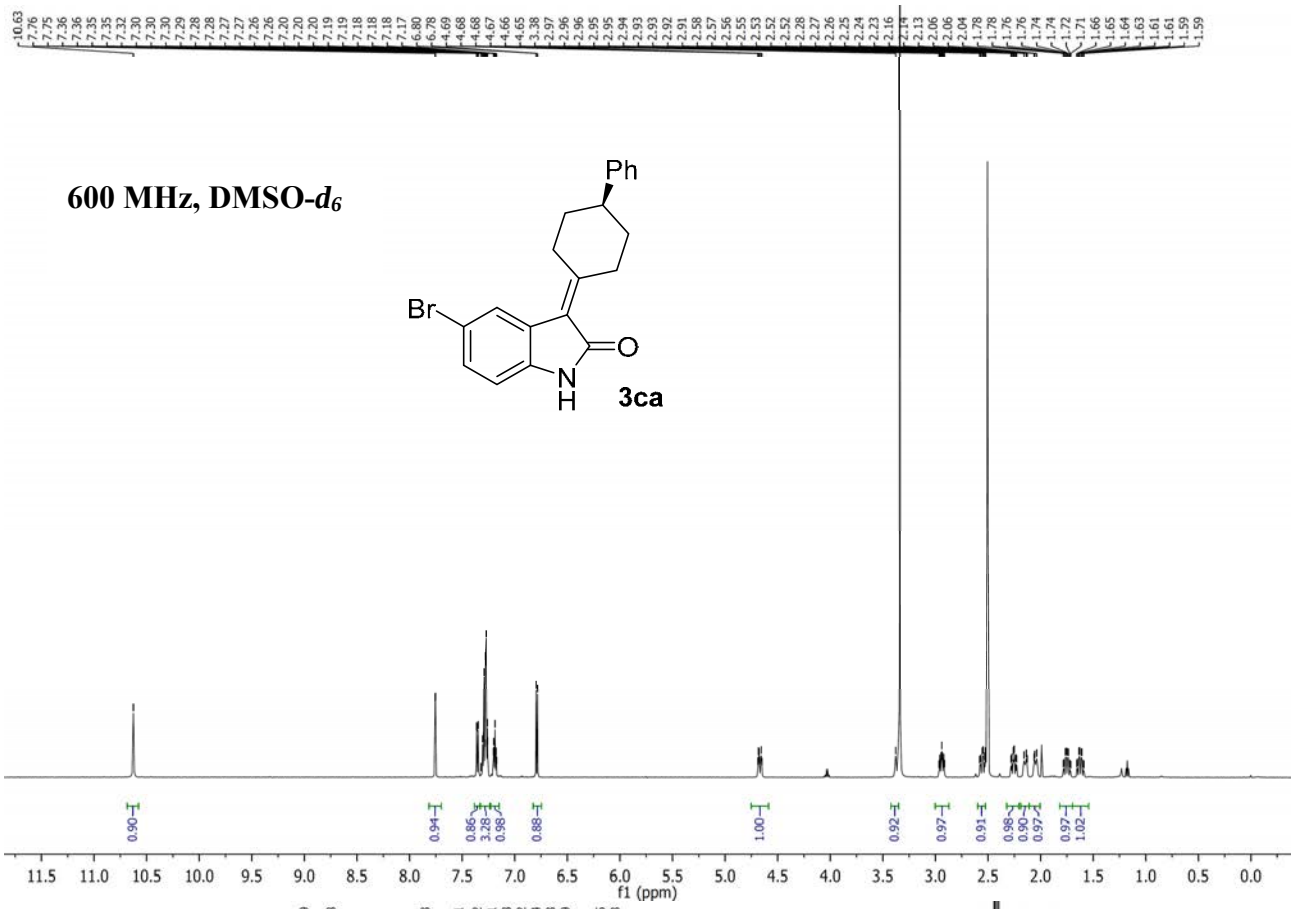


75 MHz, DMSO-*d*$_6$

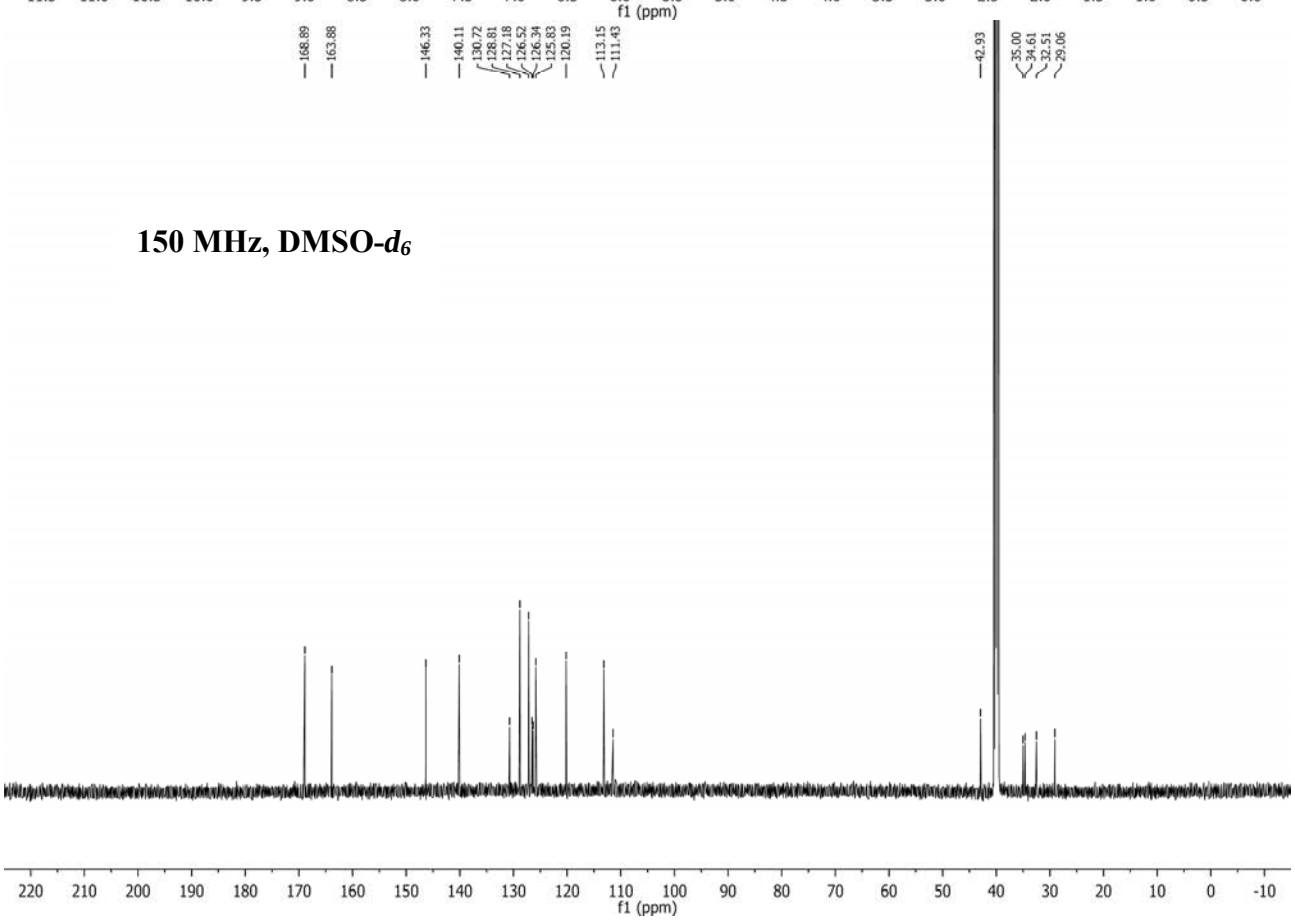


600 MHz, DMSO-d_6

3ca

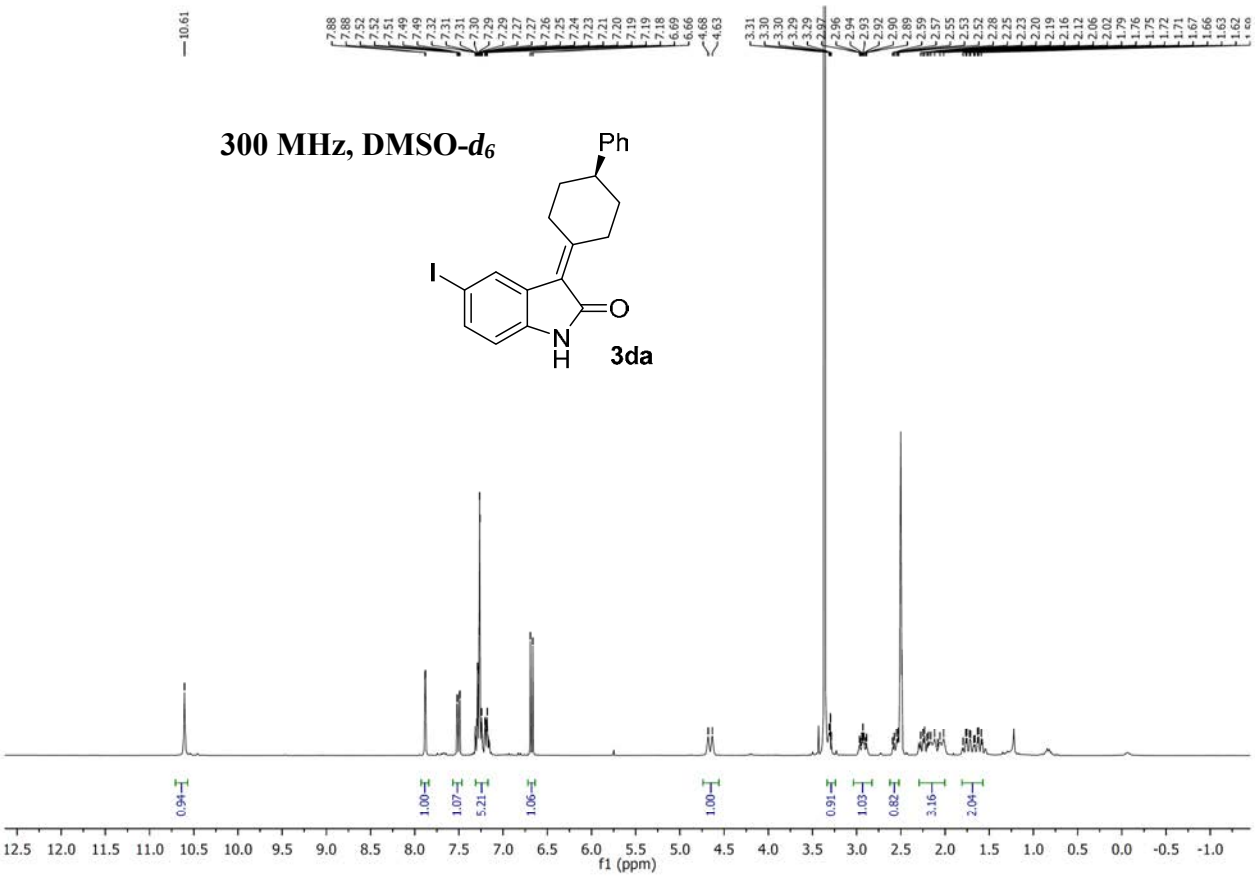


150 MHz, DMSO-d_6

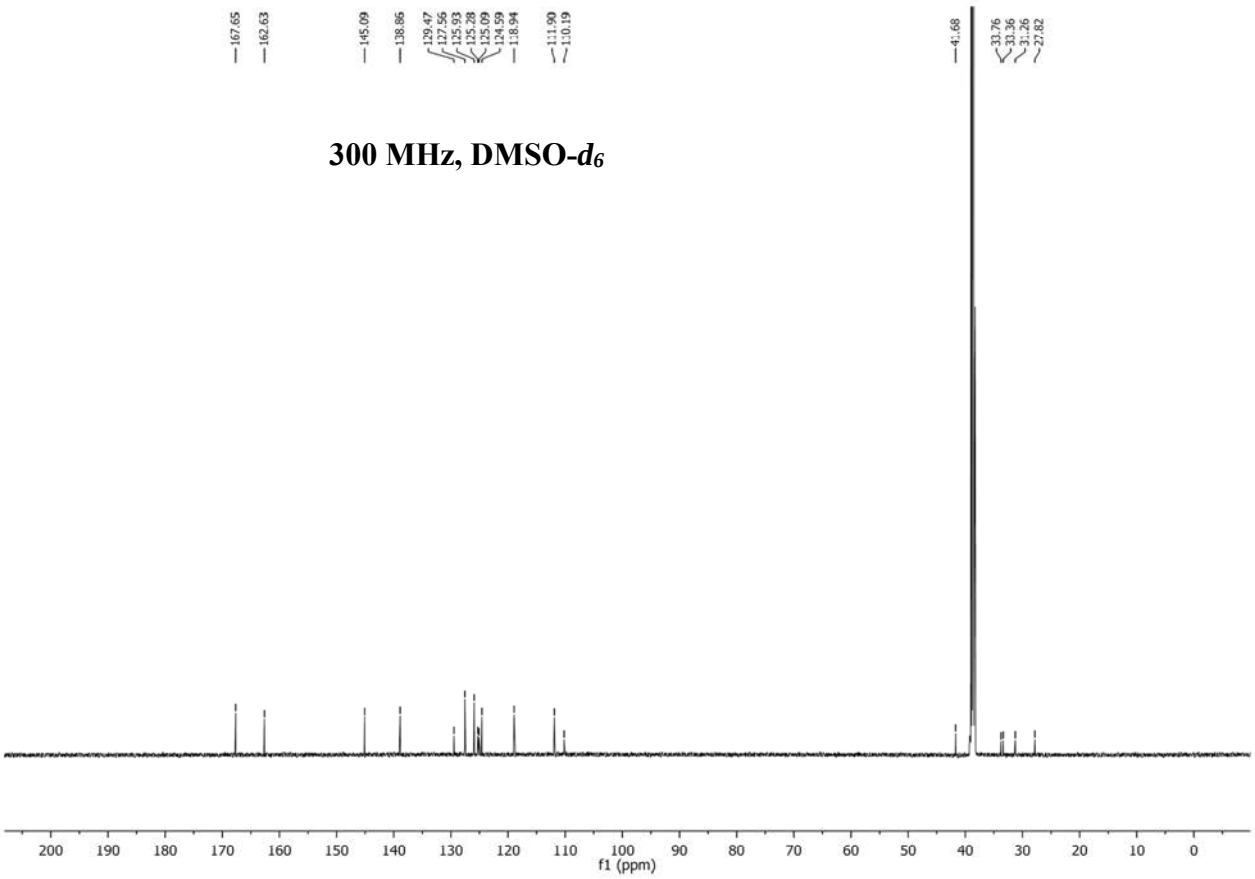


300 MHz, DMSO-*d*$_6$

3da

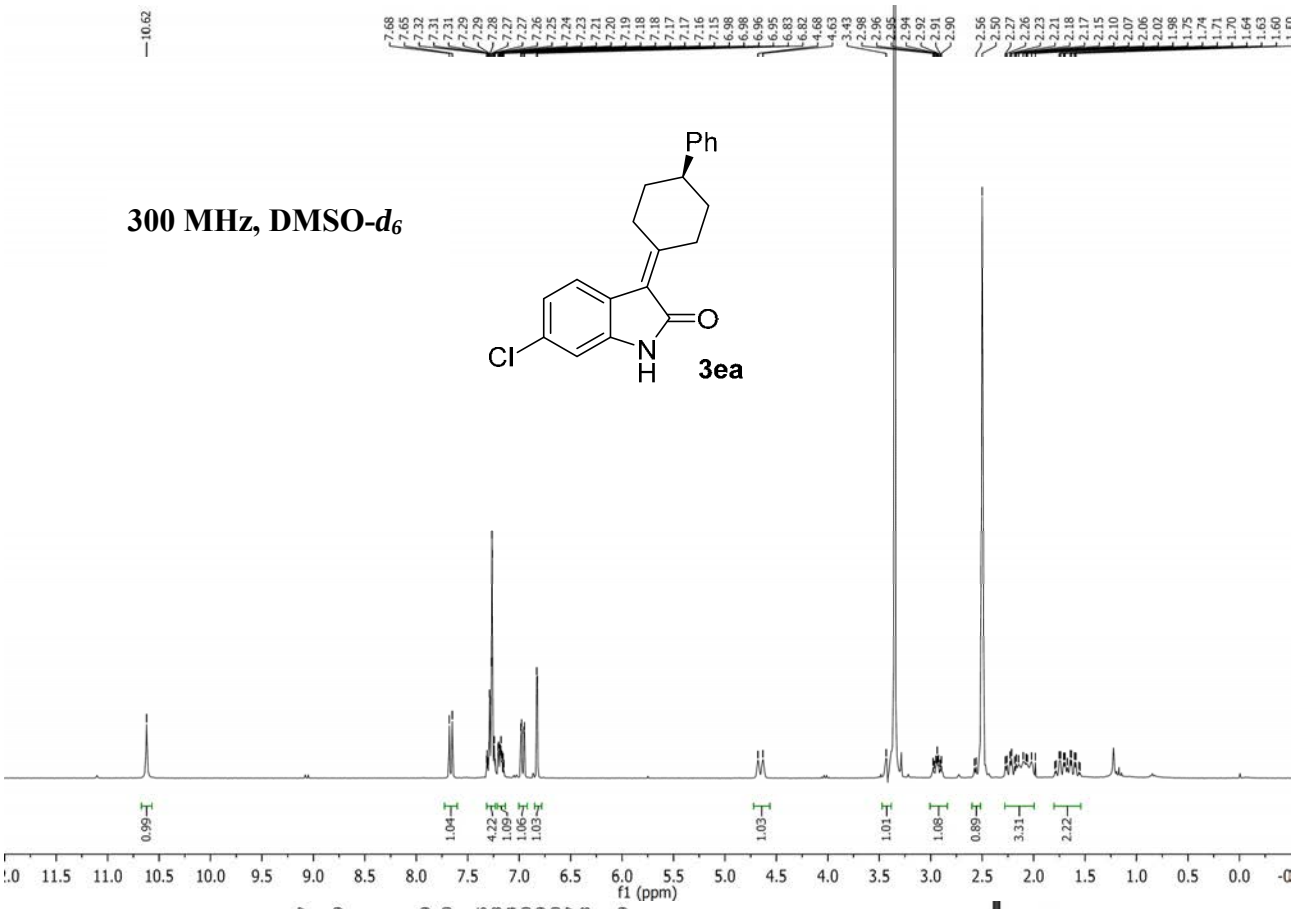


300 MHz, DMSO-*d*$_6$

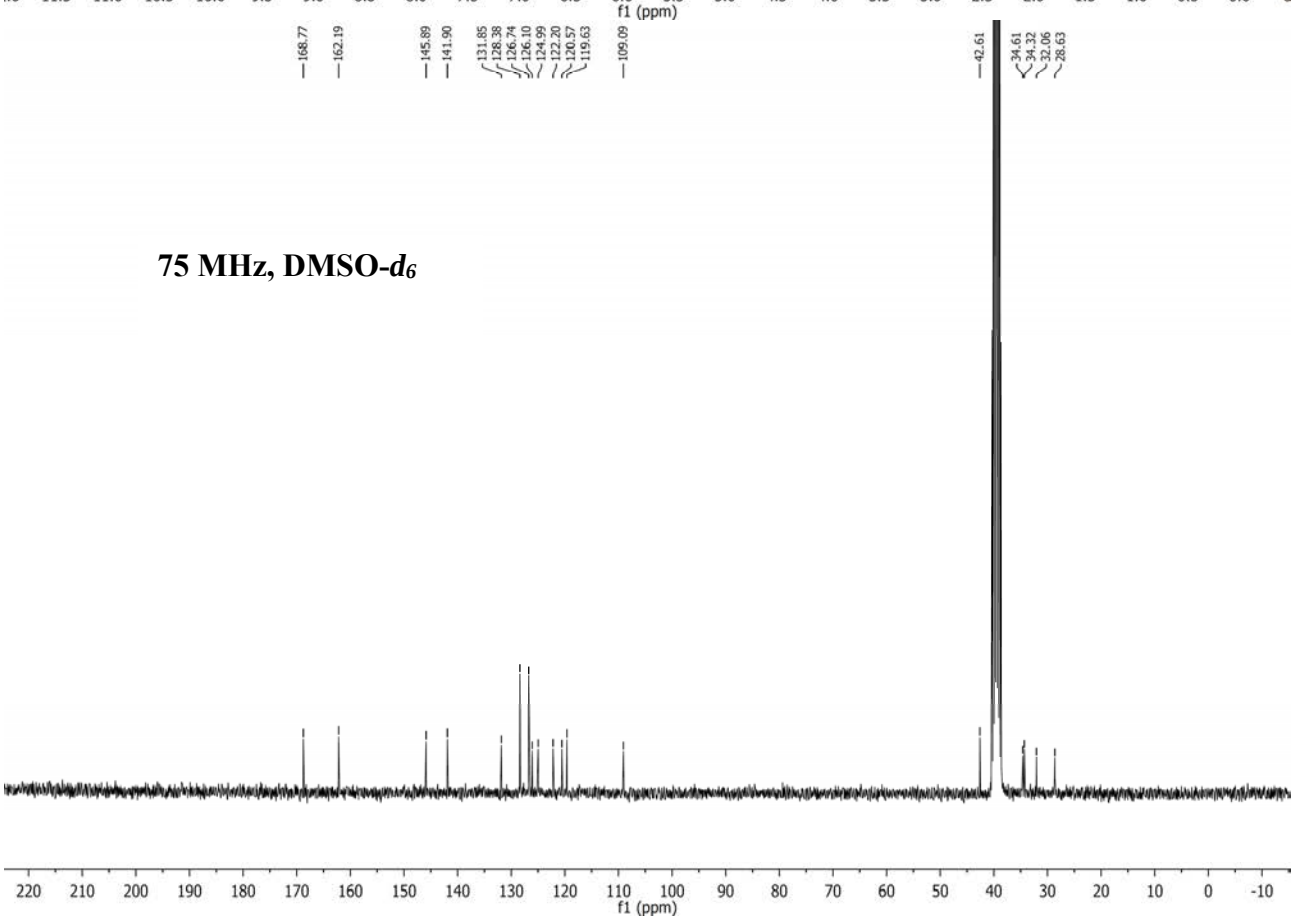


300 MHz, DMSO-*d*$_6$

3ea

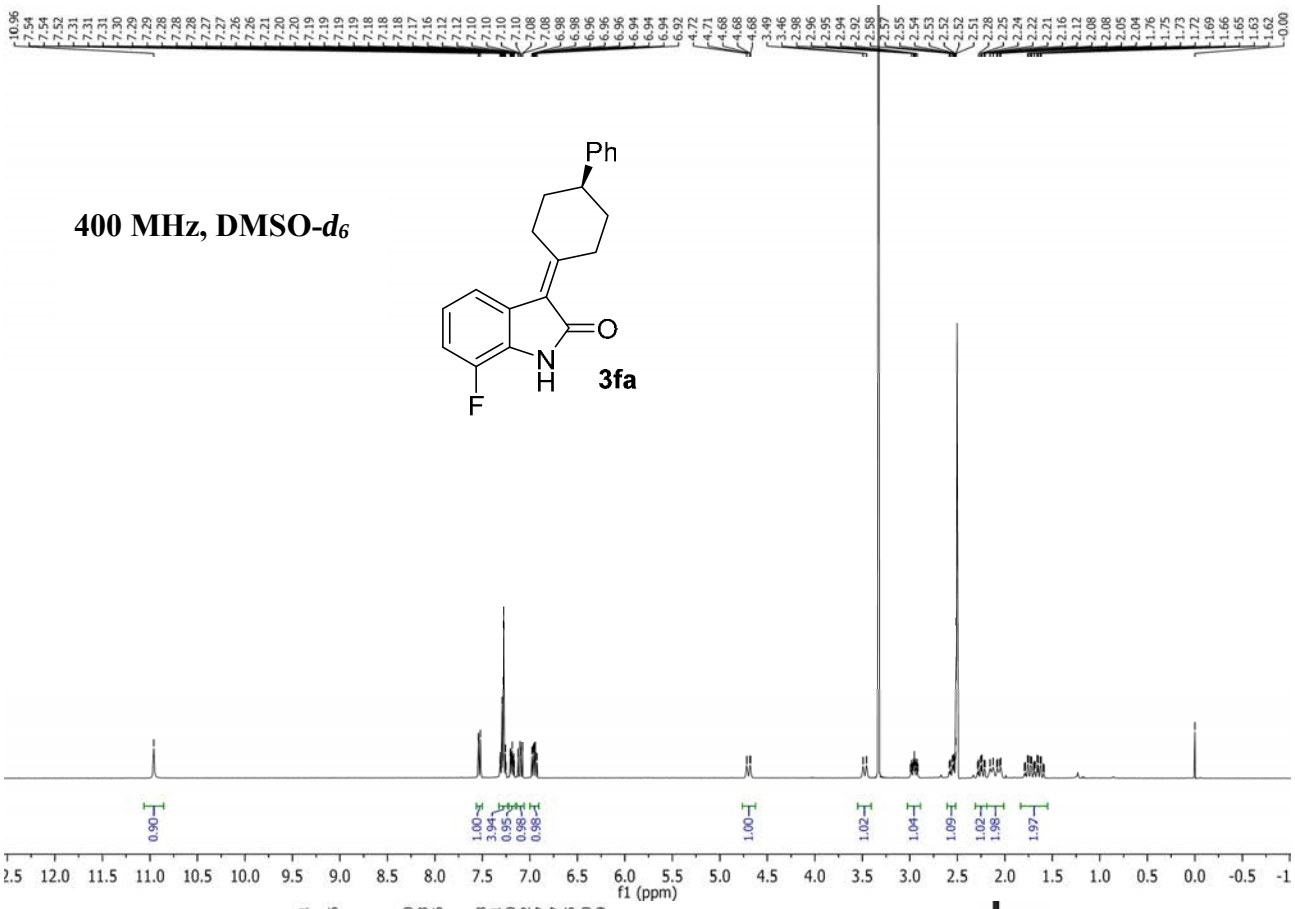


75 MHz, DMSO-*d*$_6$

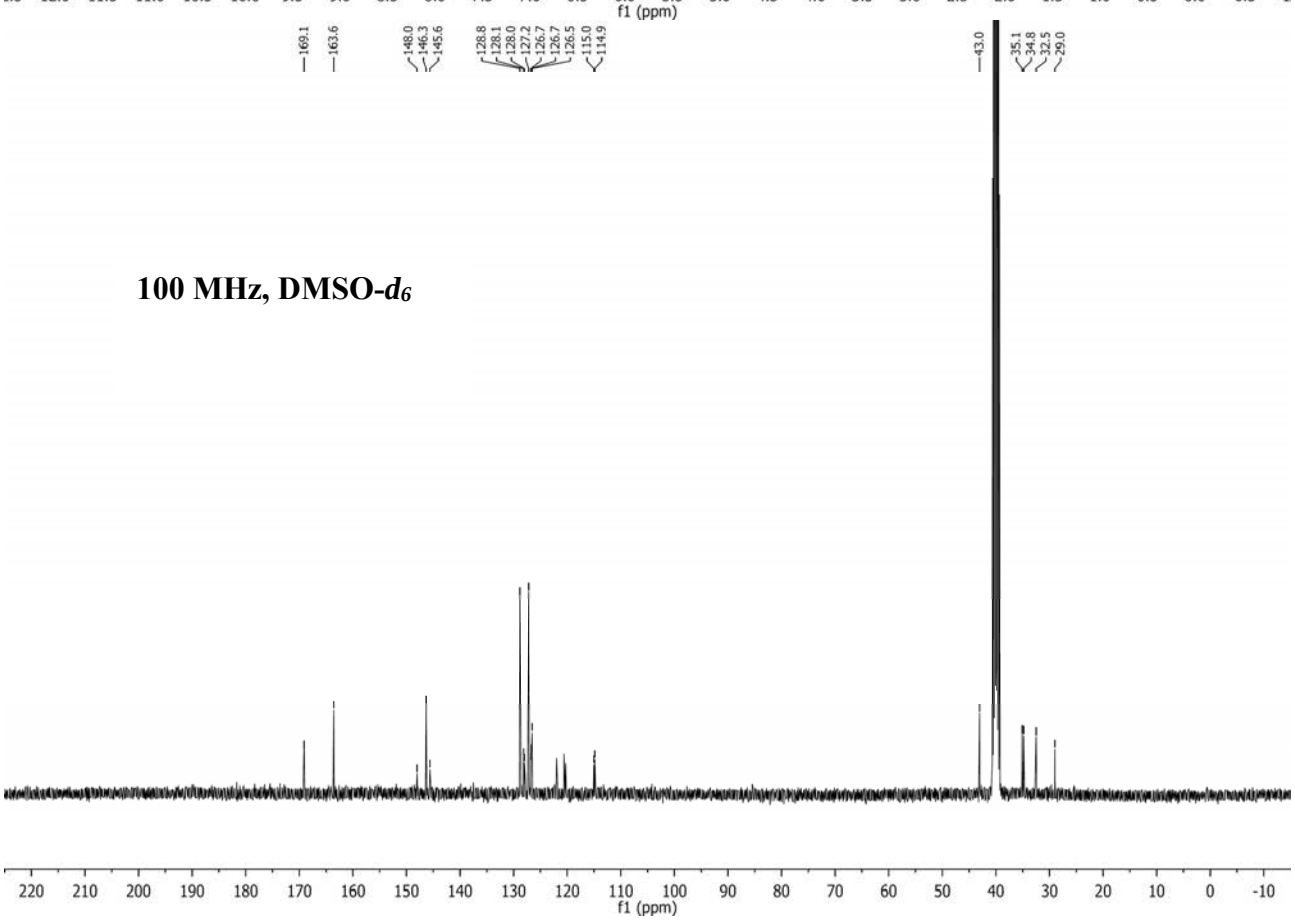


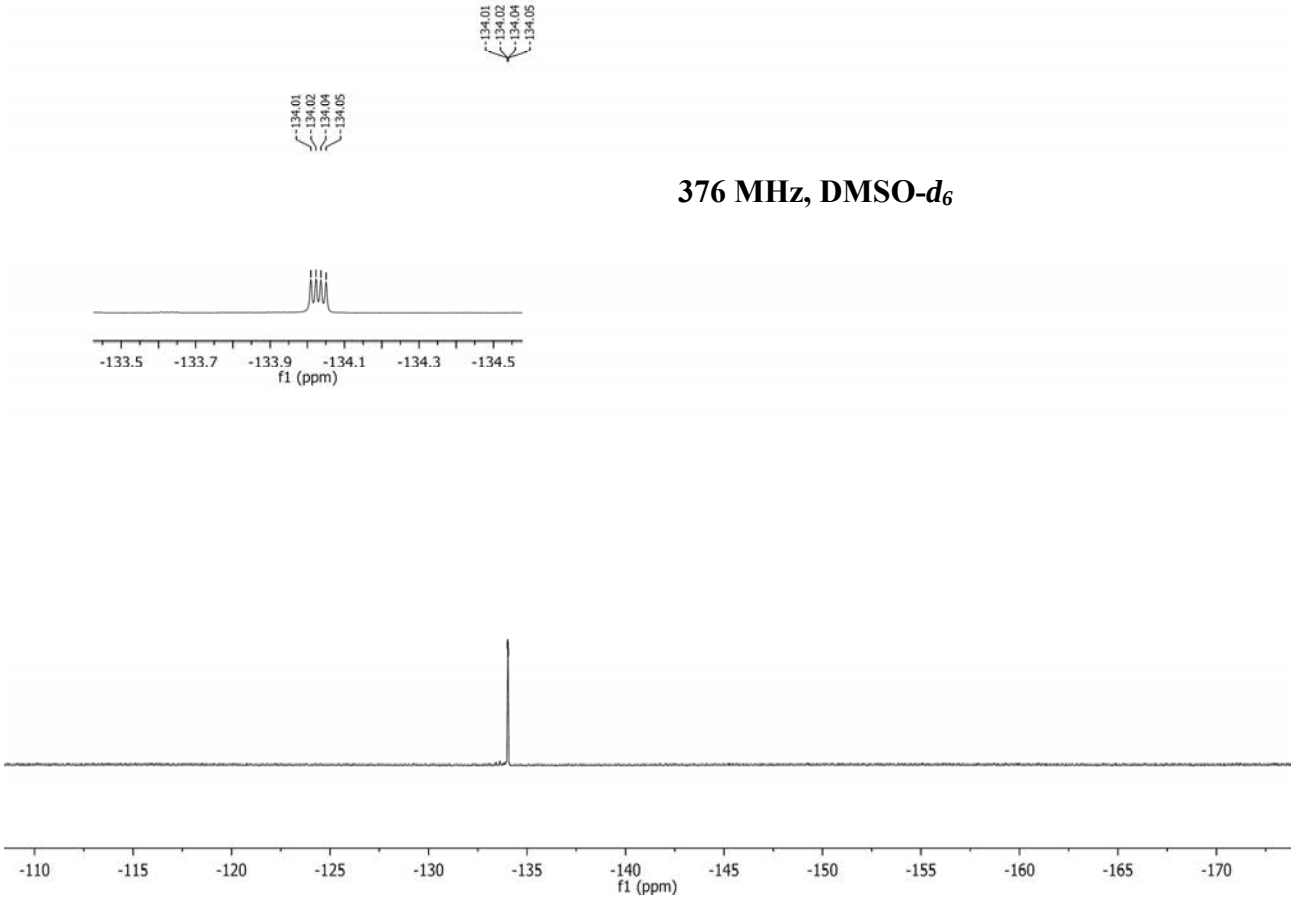
400 MHz, DMSO-*d6*

3fa



100 MHz, DMSO-*d6*

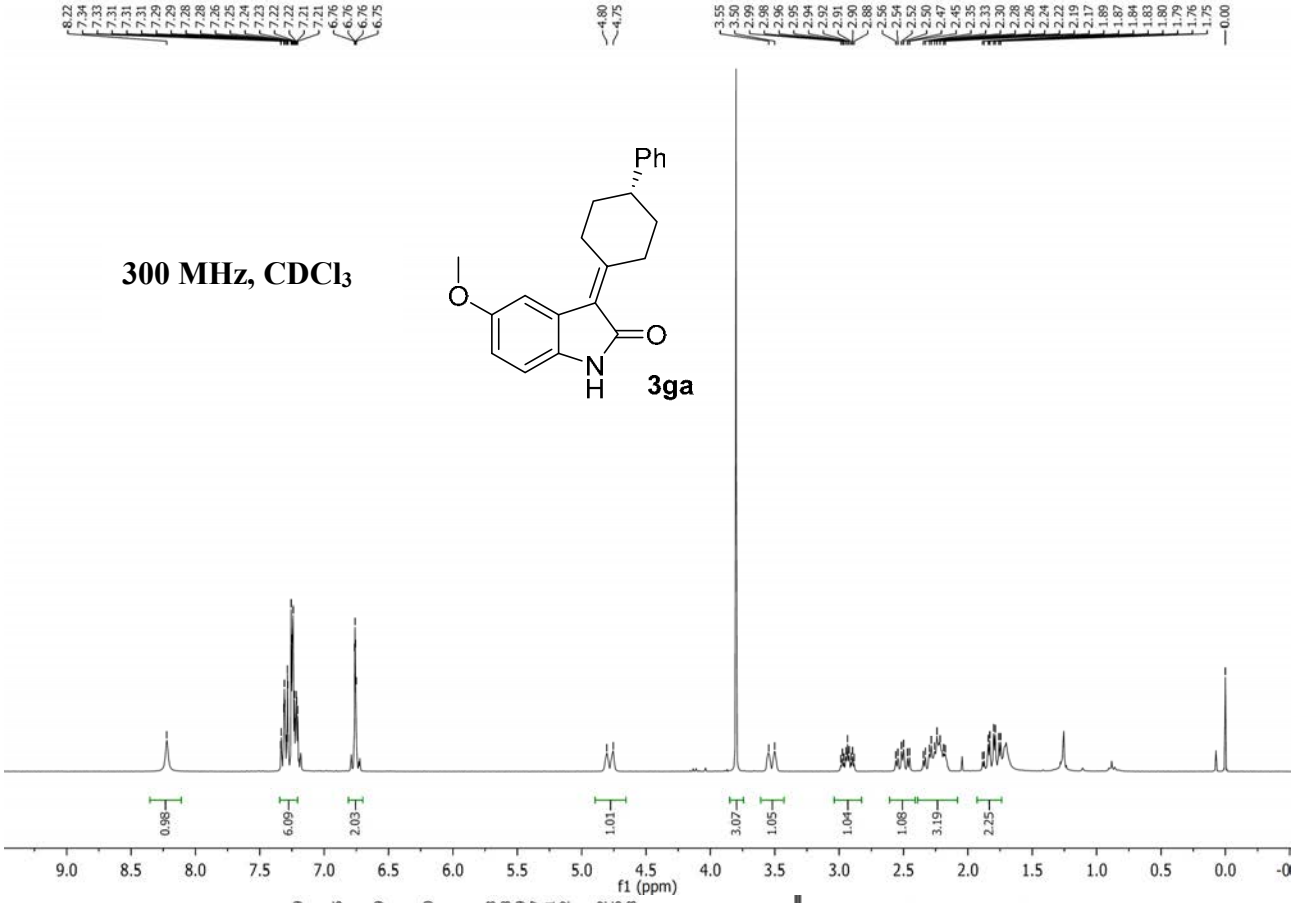




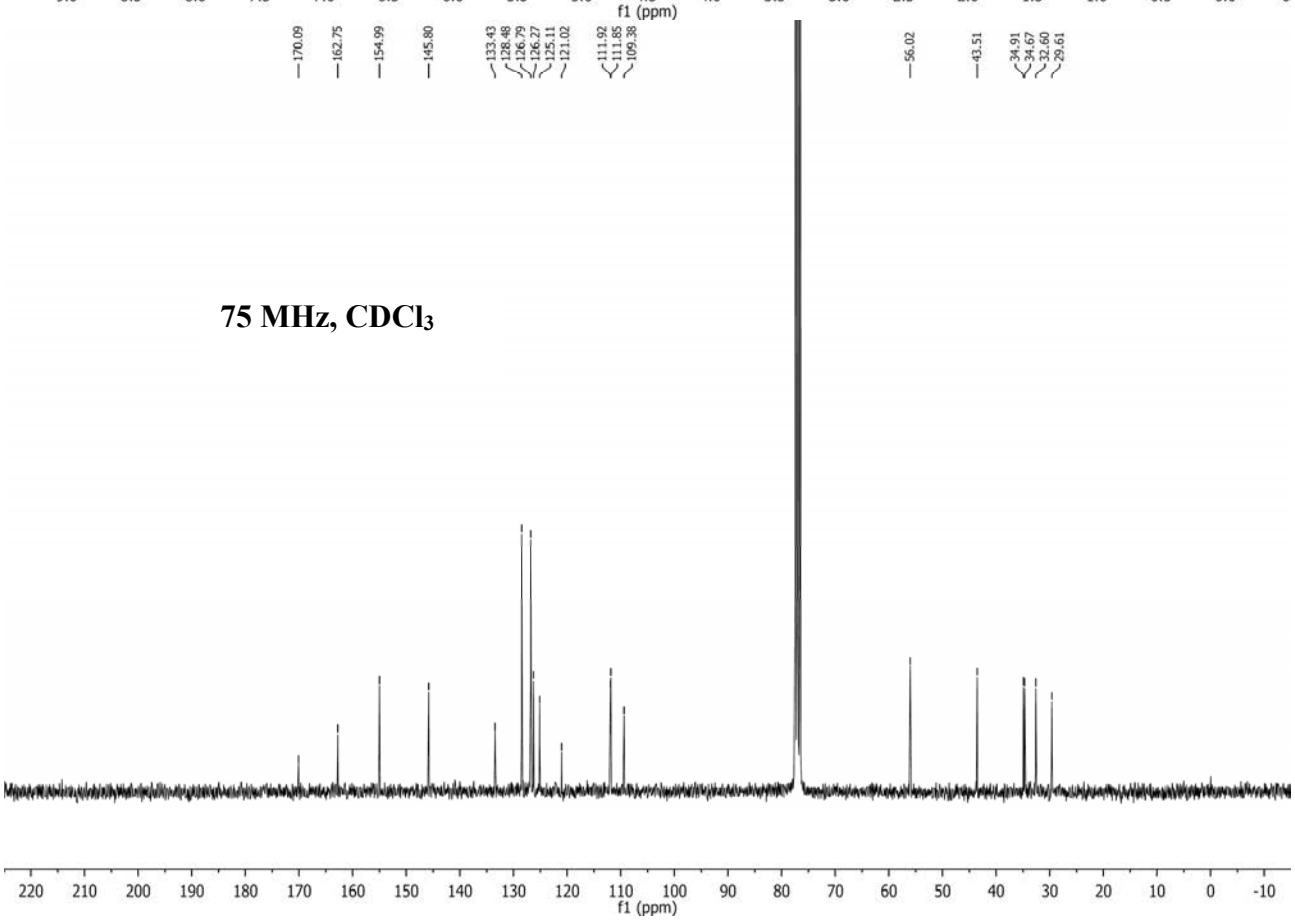
376 MHz, DMSO-d_6

300 MHz, $CDCl_3$

3ga

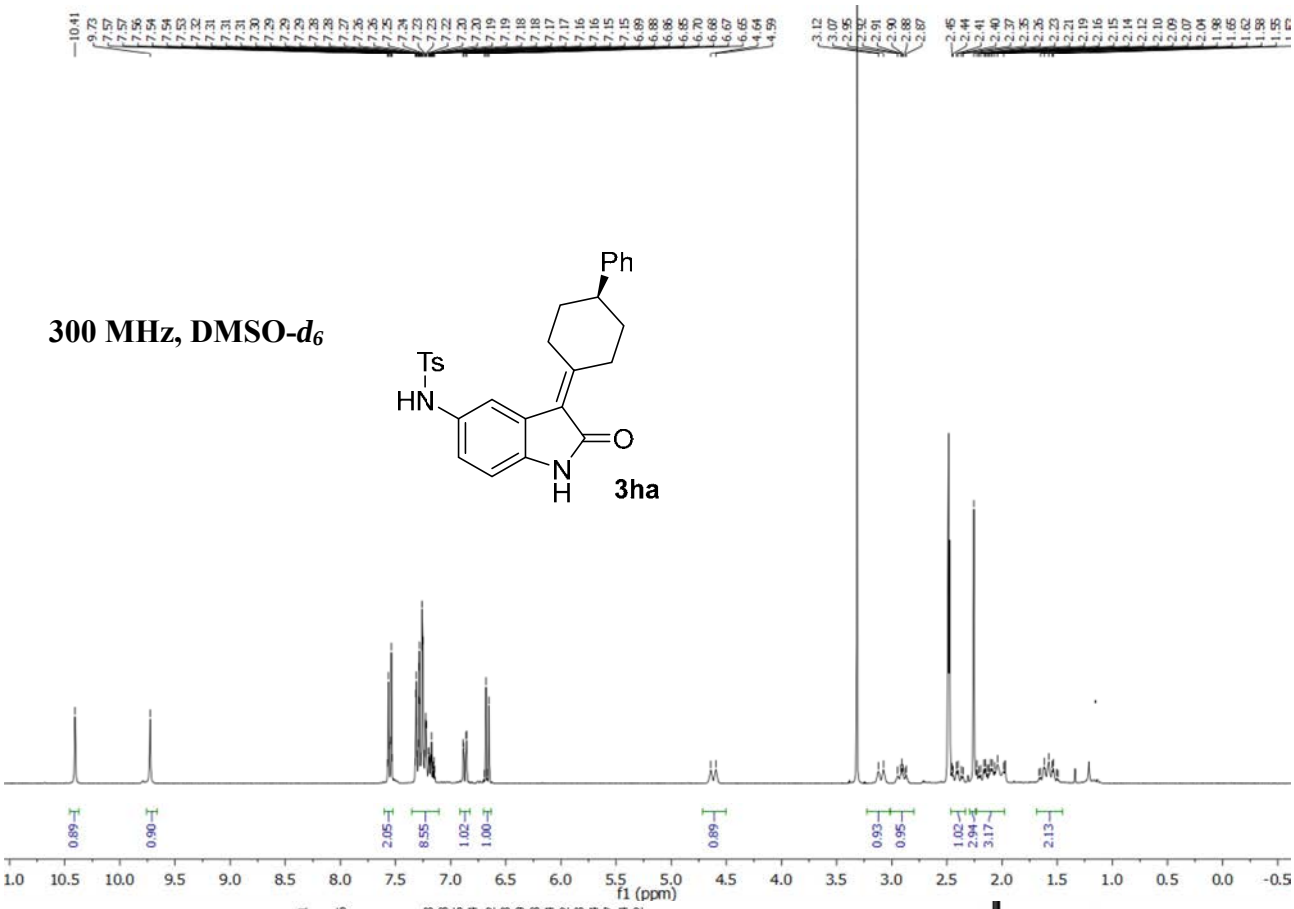


75 MHz, $CDCl_3$

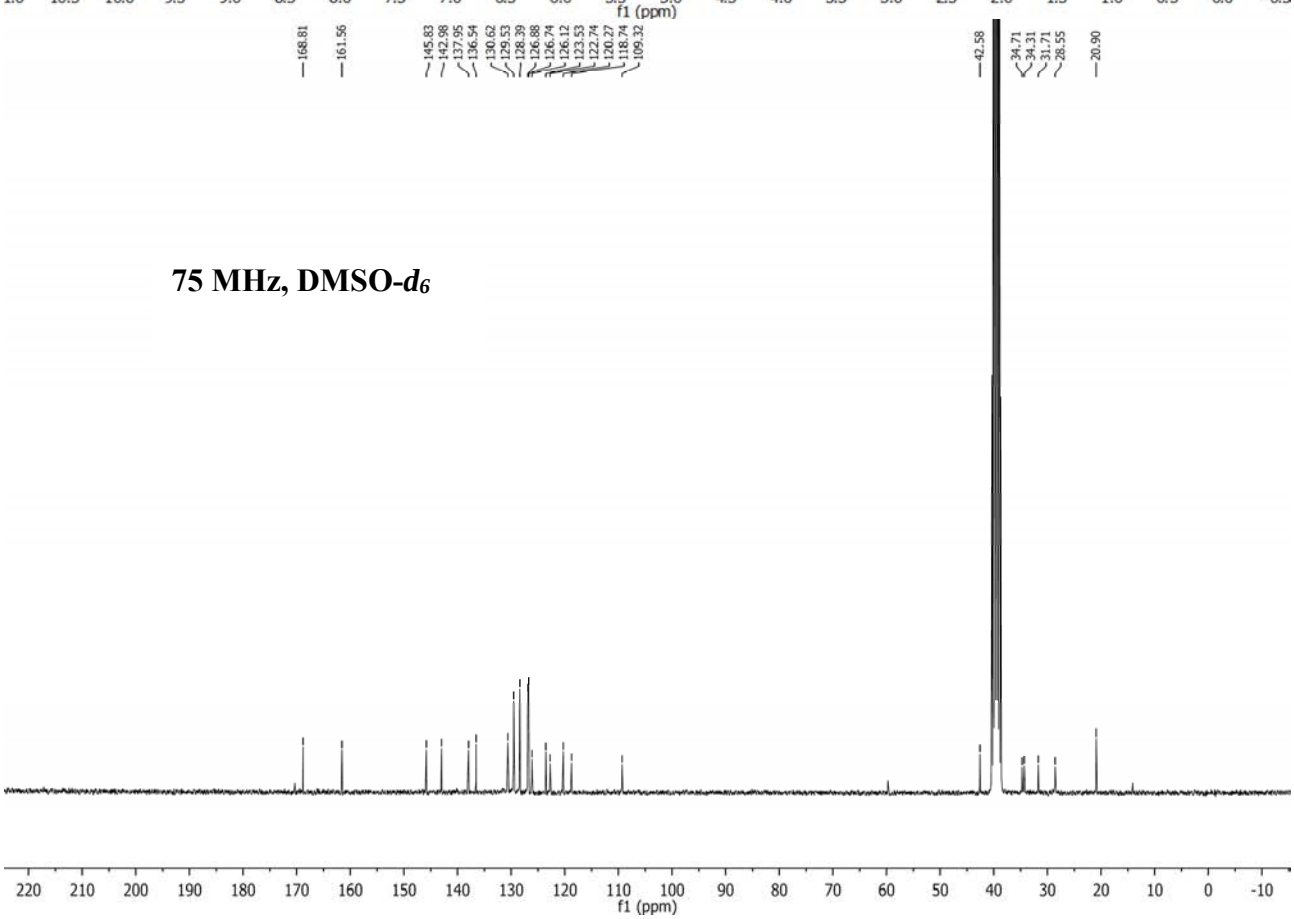


300 MHz, DMSO-*d*$_6$

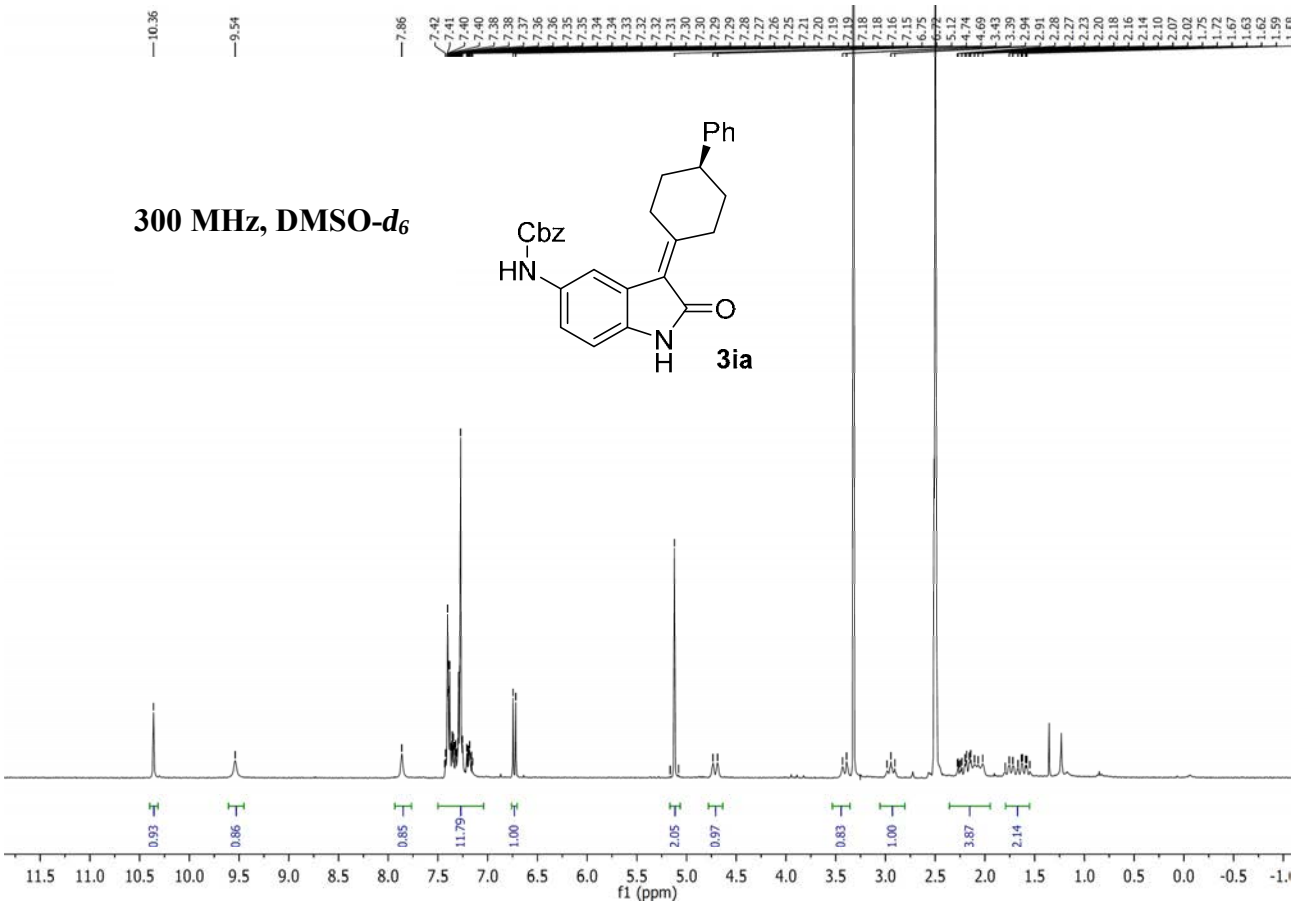
3ha



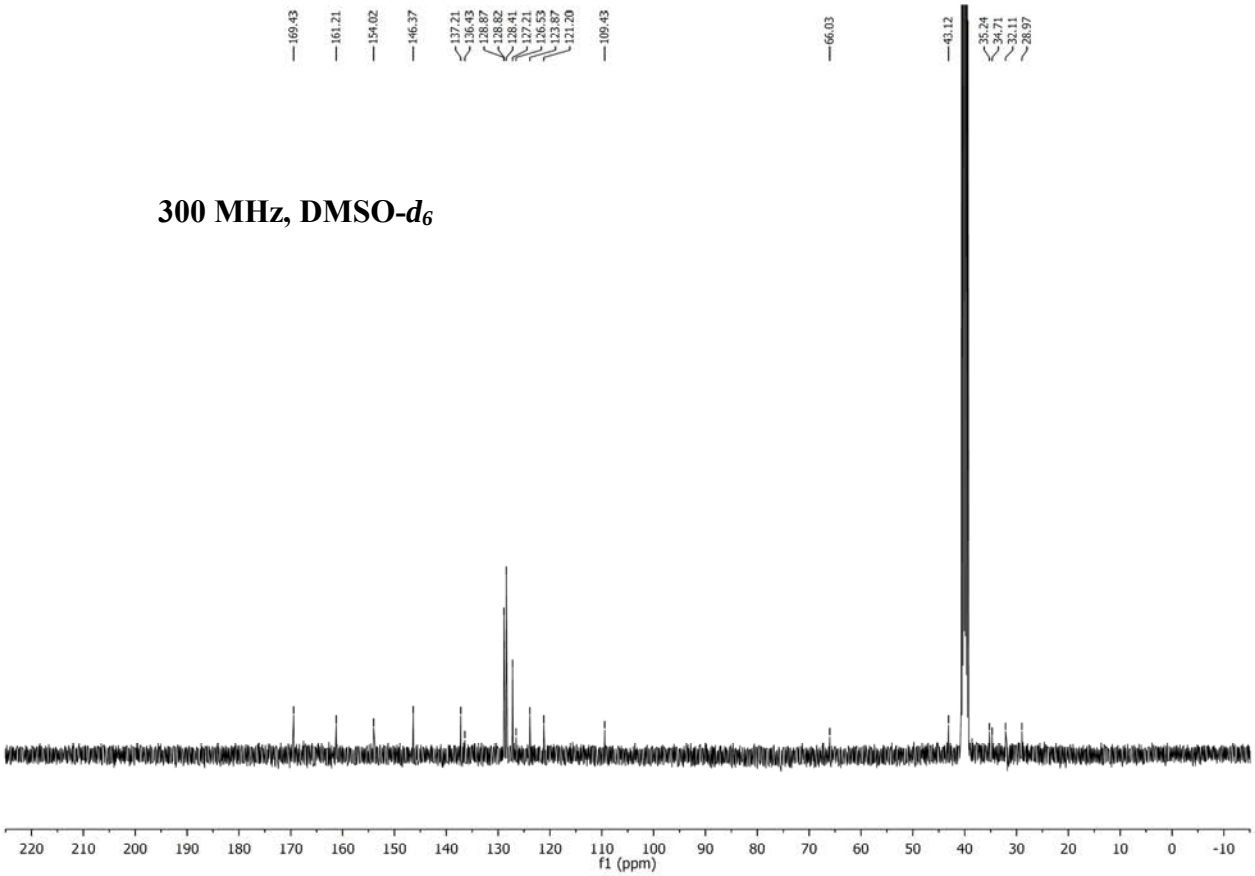
75 MHz, DMSO-*d*$_6$



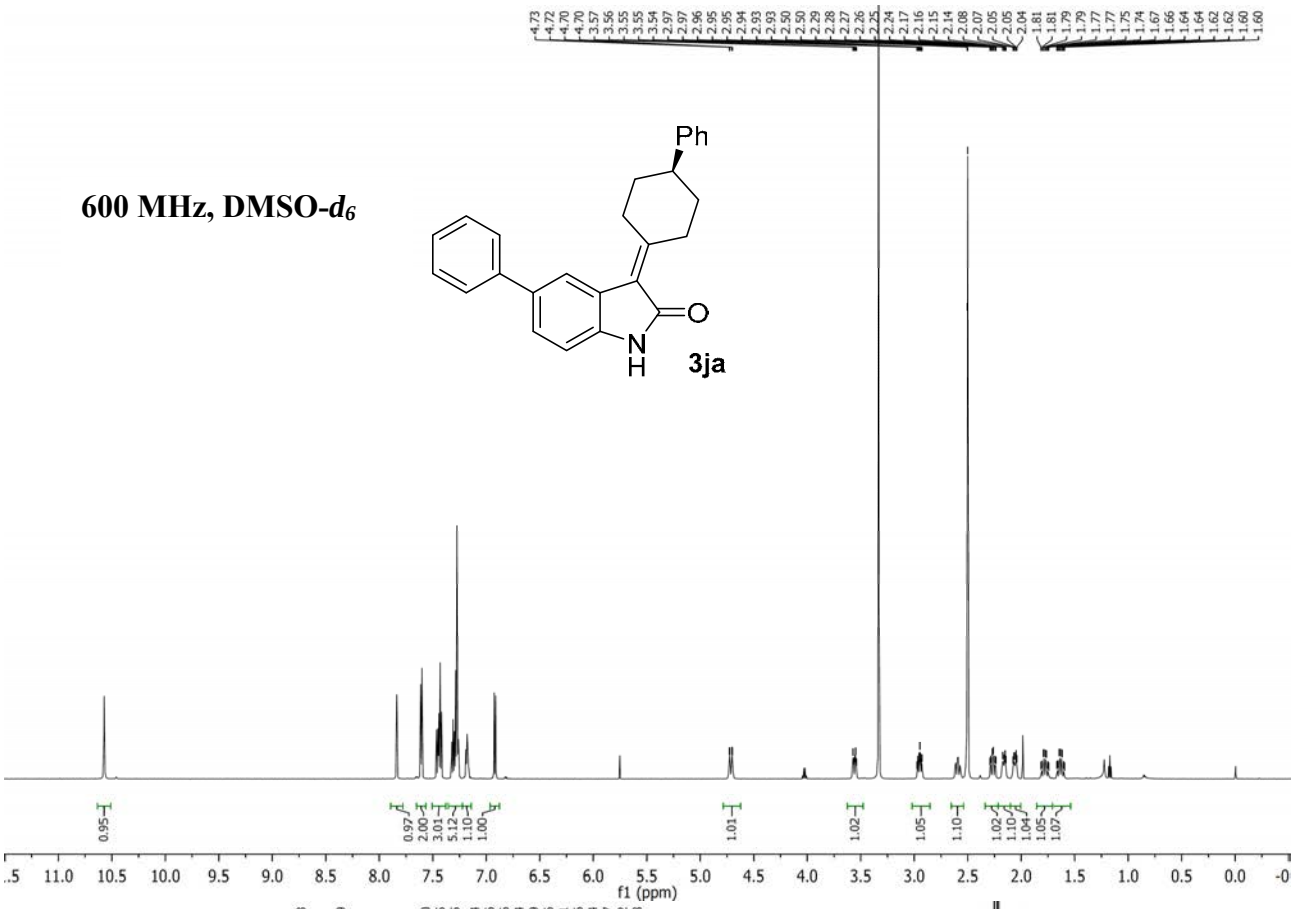
300 MHz, DMSO-*d*$_6$



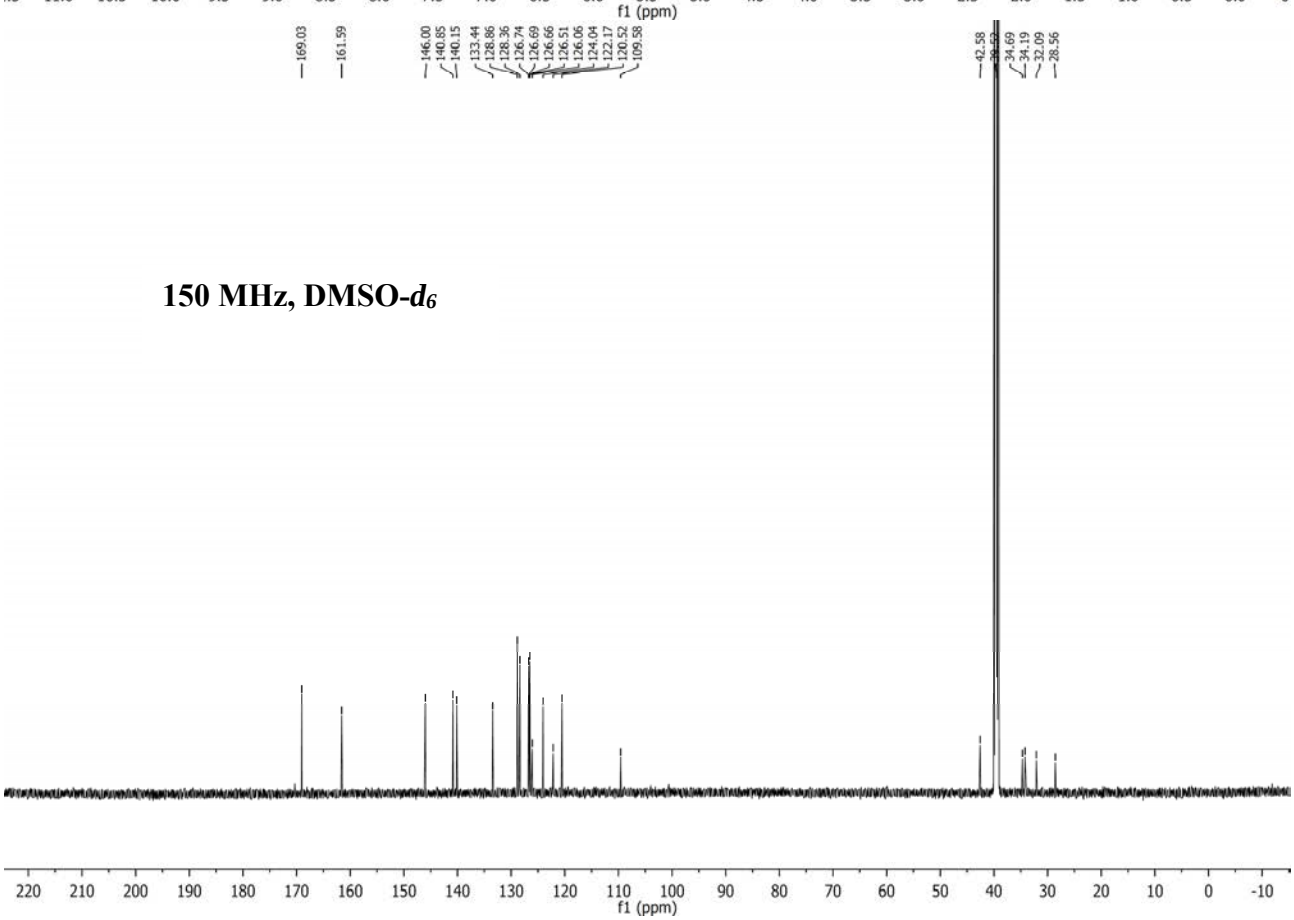
300 MHz, DMSO-*d*$_6$



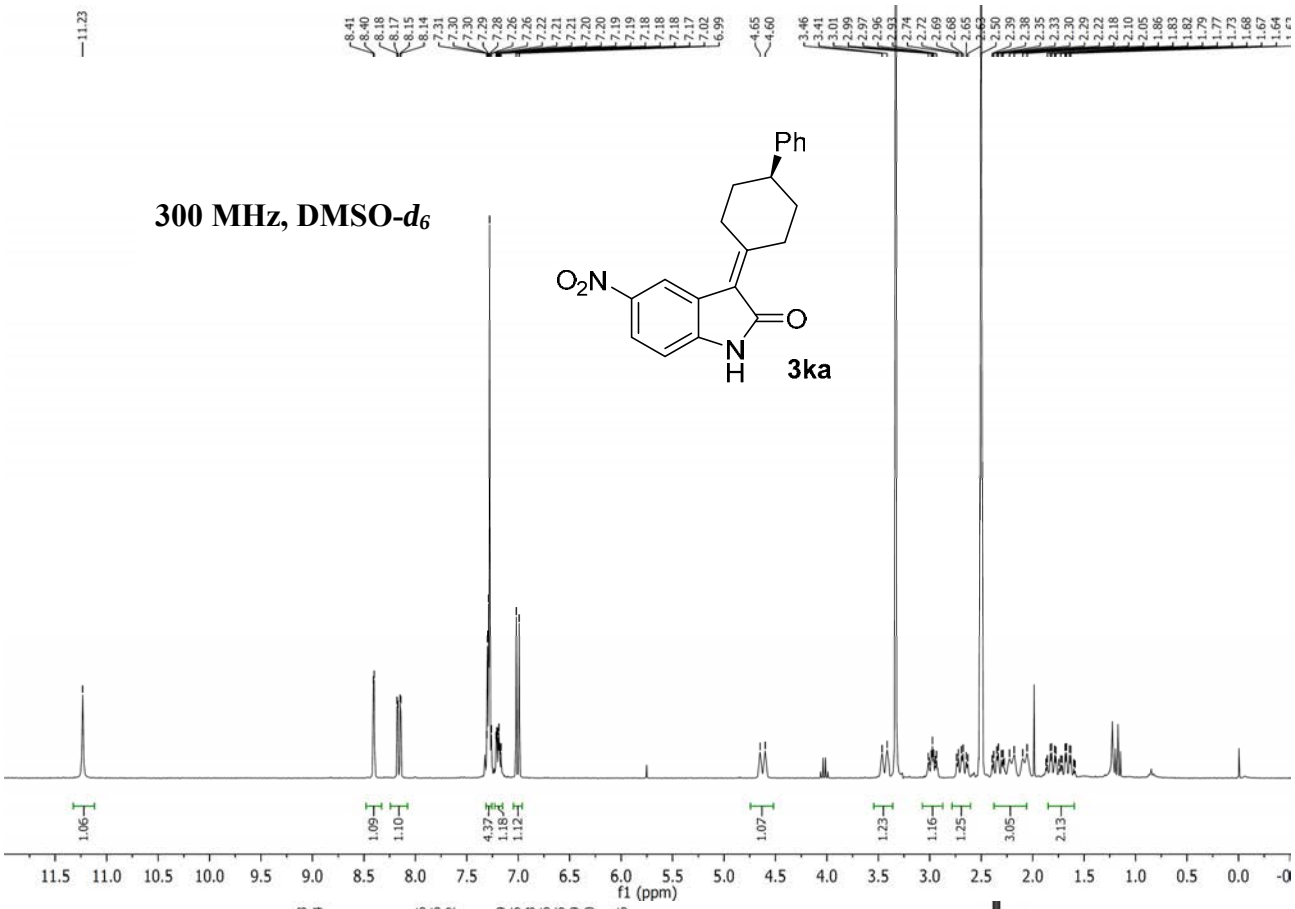
600 MHz, DMSO-*d6*



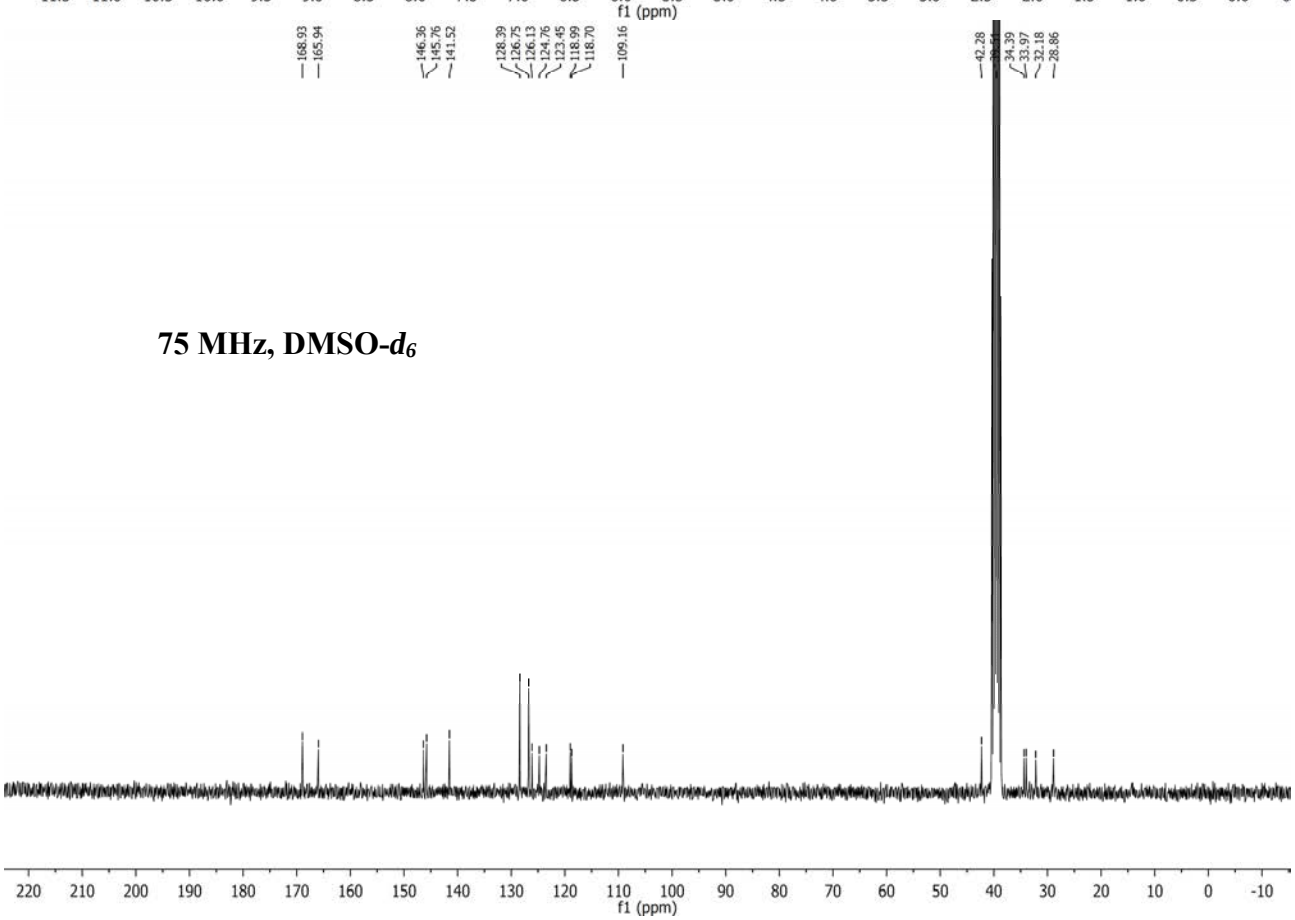
150 MHz, DMSO-*d6*



300 MHz, DMSO-*d*$_6$

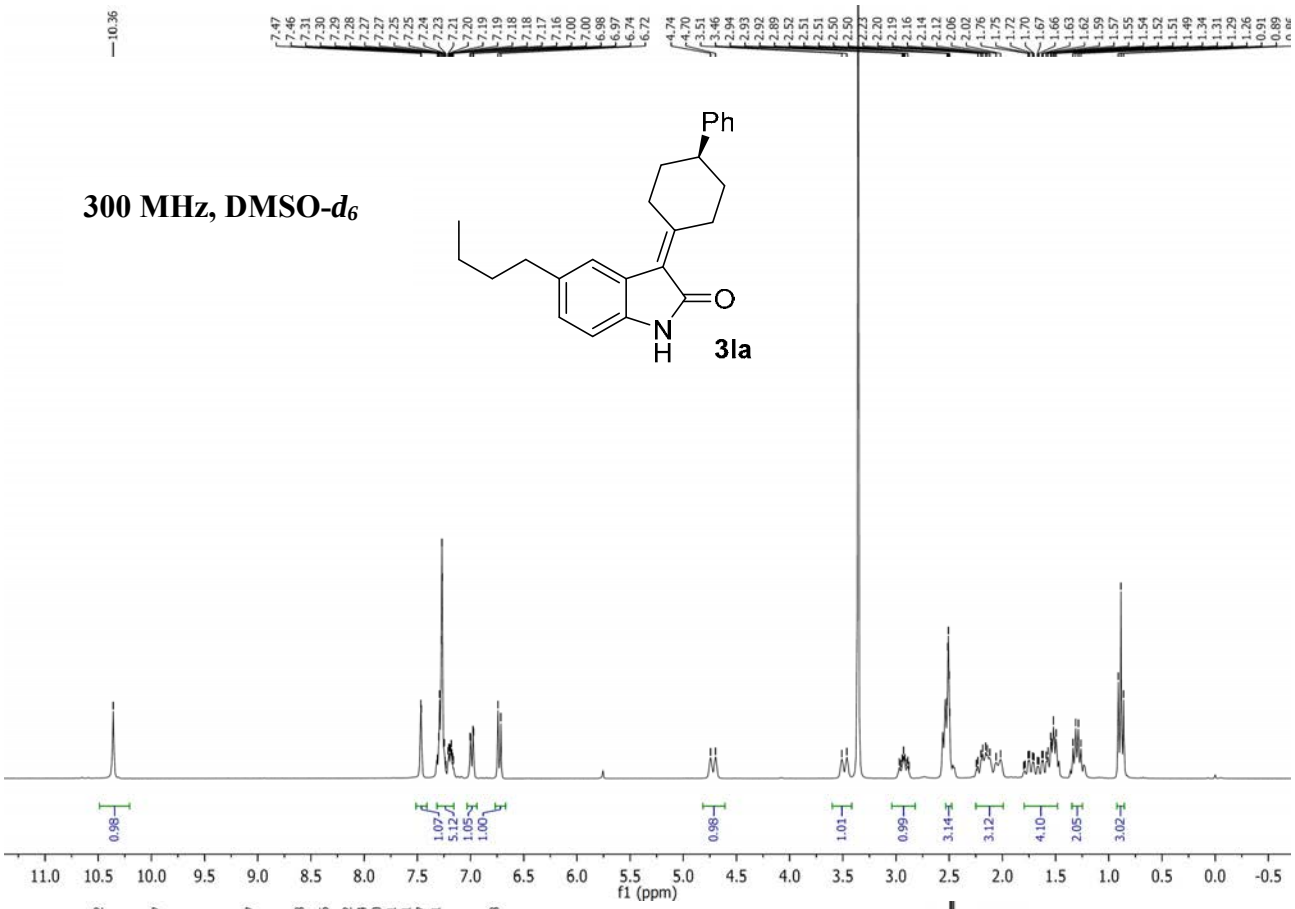


75 MHz, DMSO-*d*$_6$

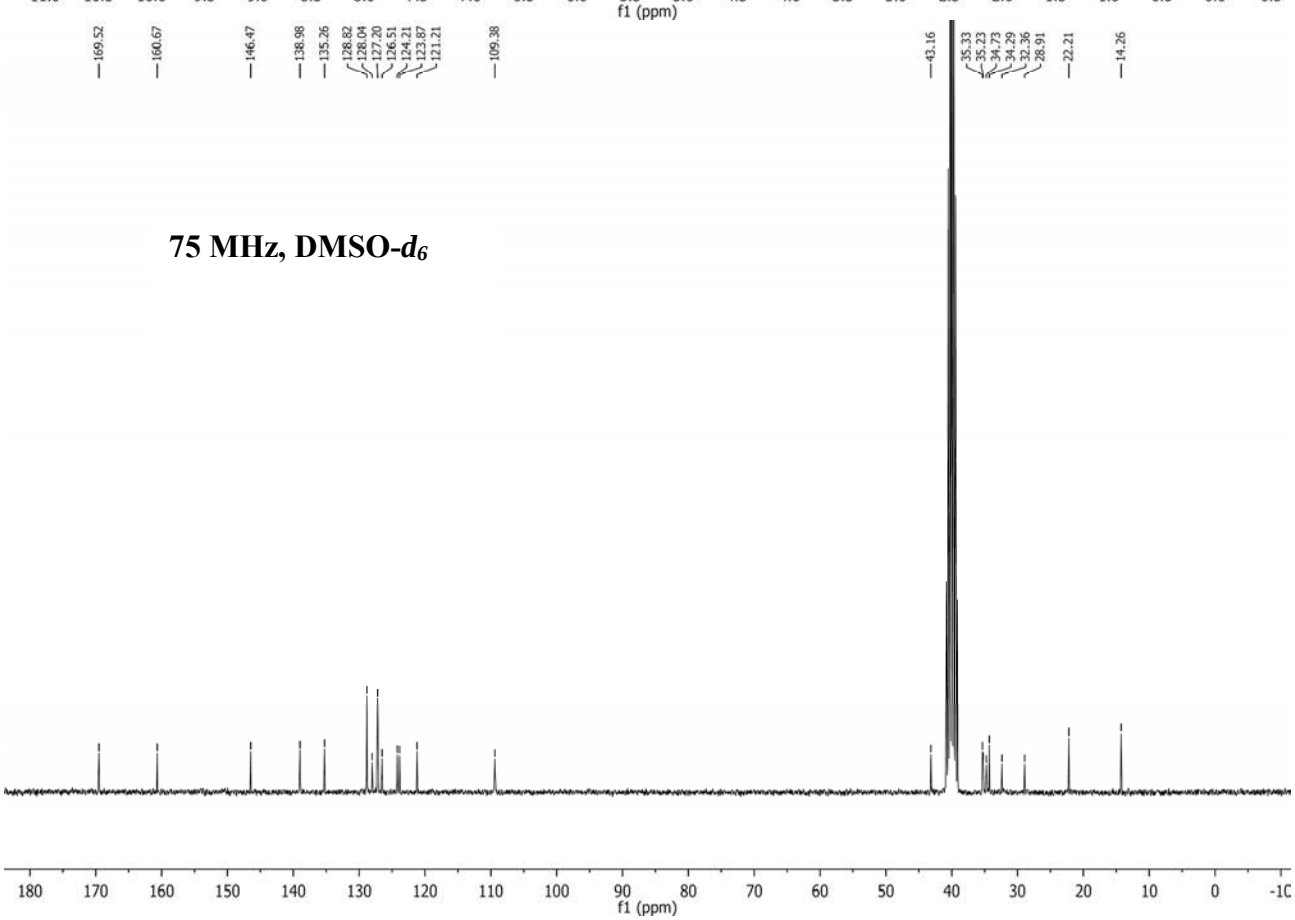


300 MHz, DMSO-*d*$_6$

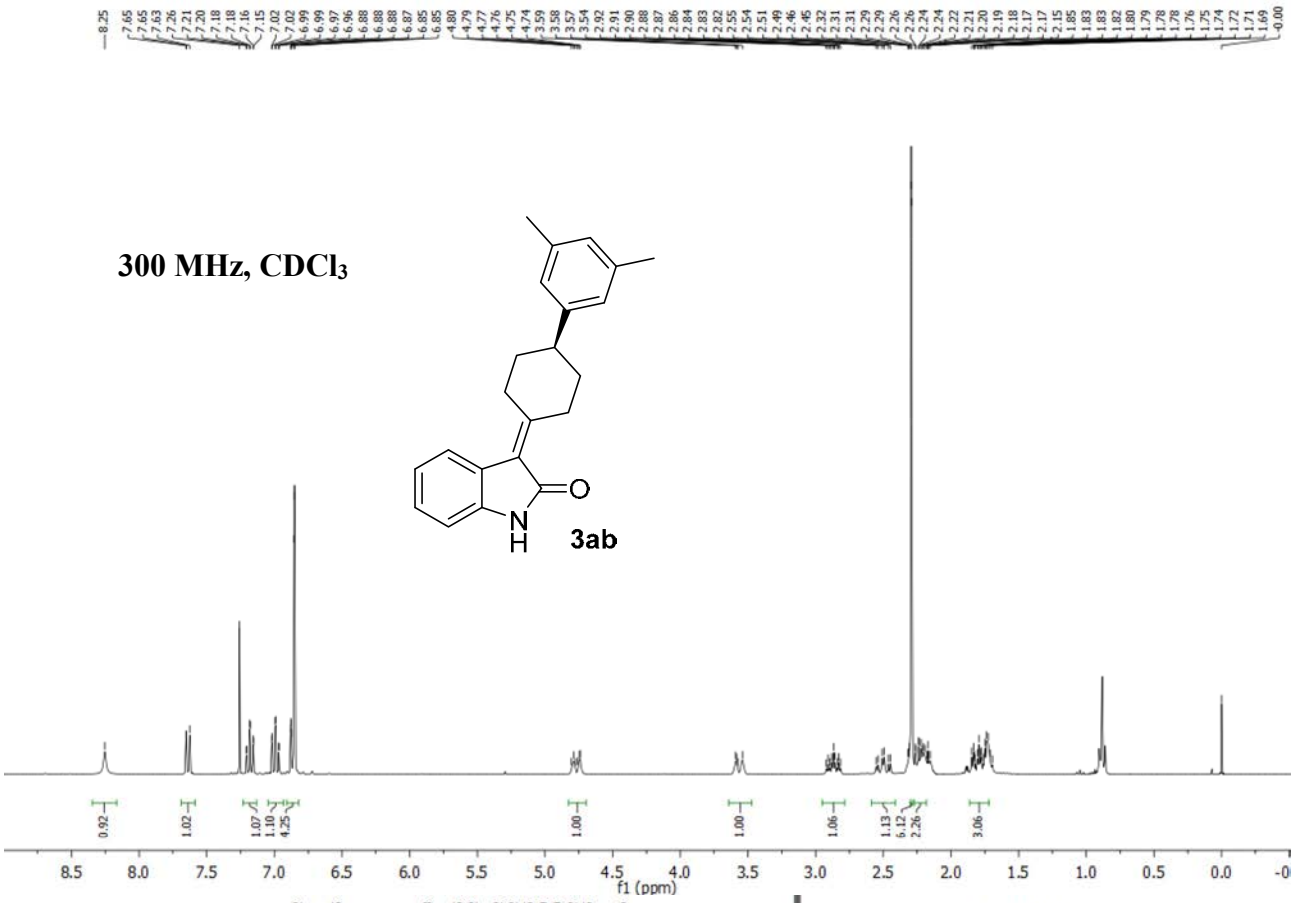
3la



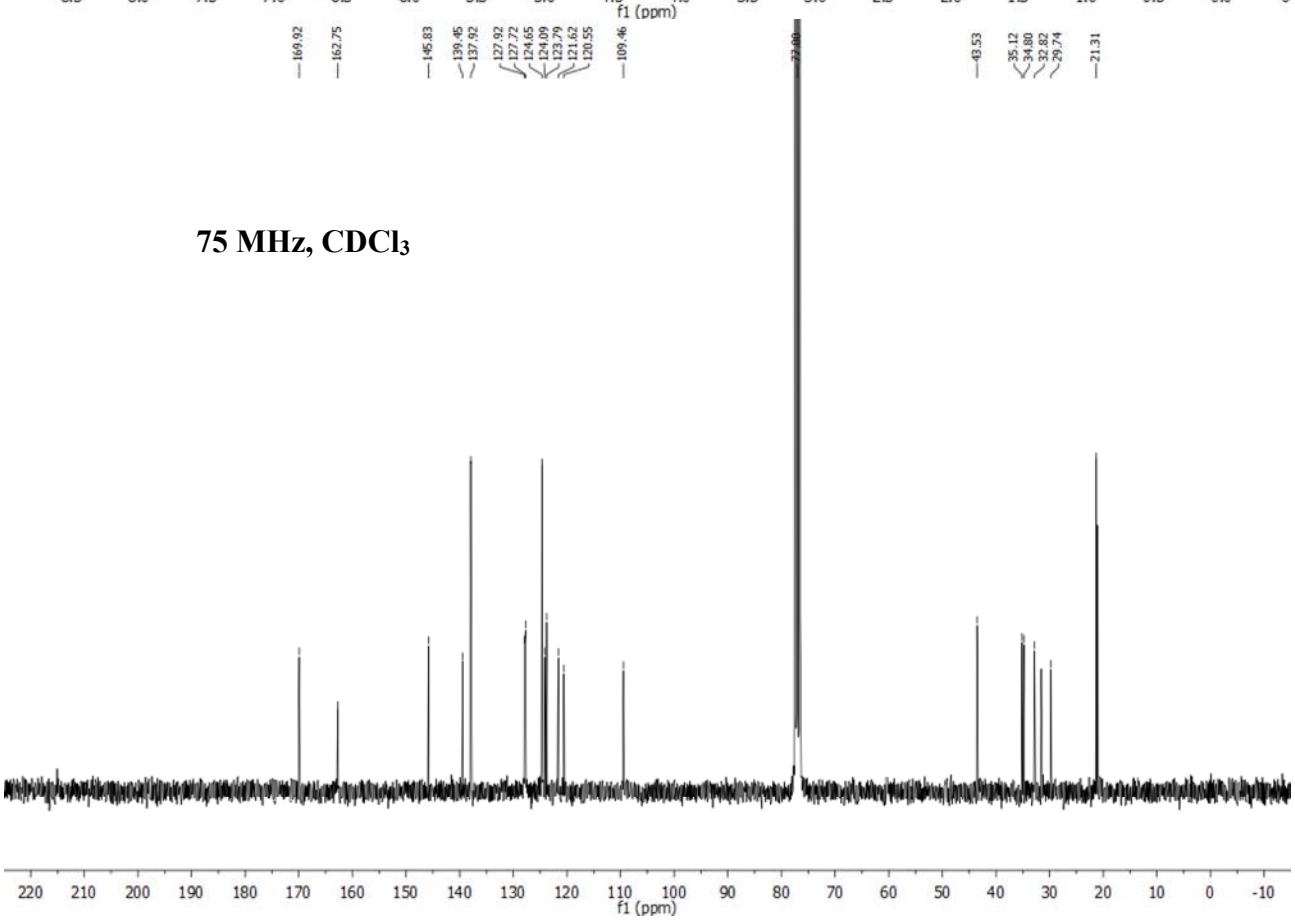
75 MHz, DMSO-*d*$_6$

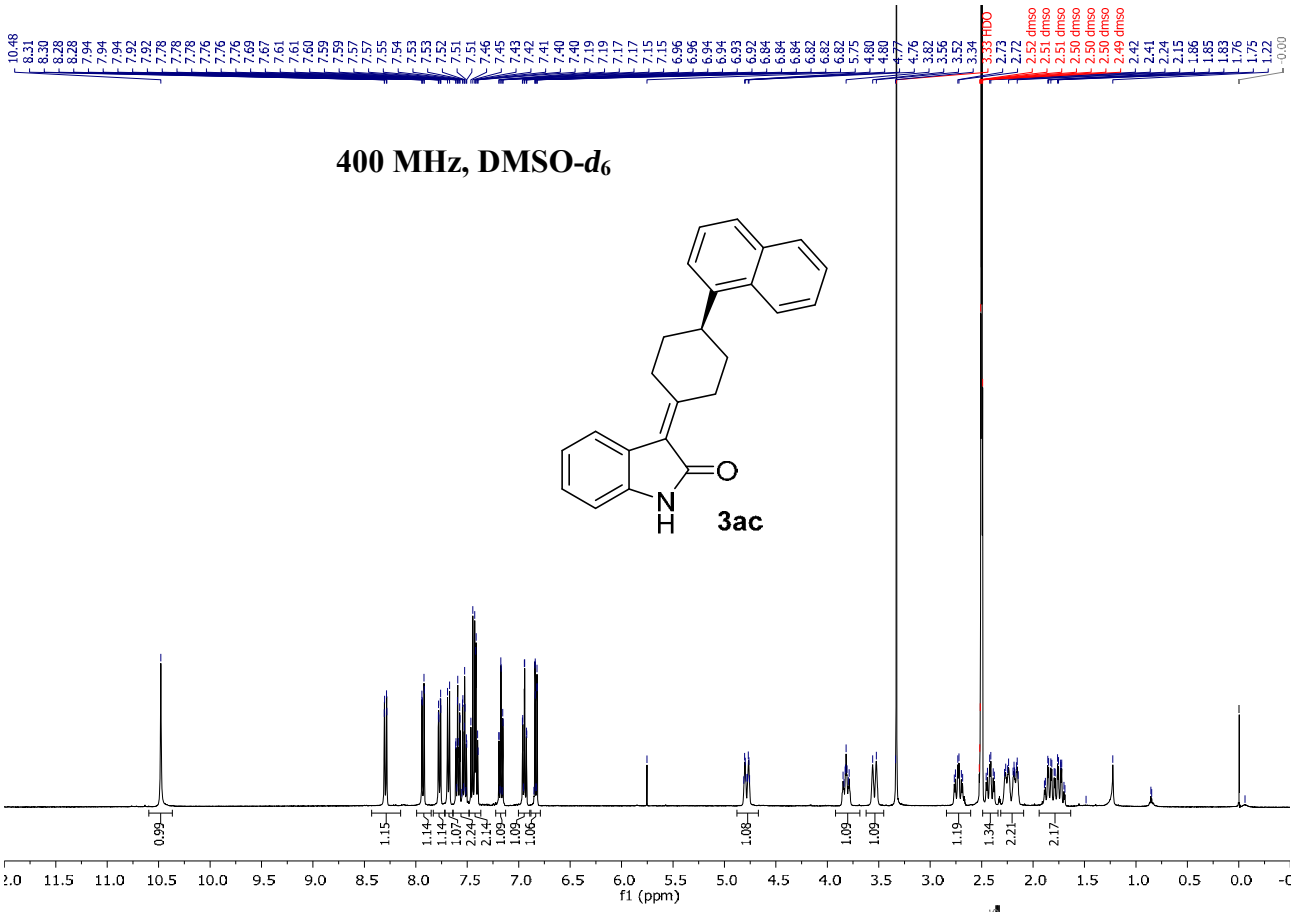


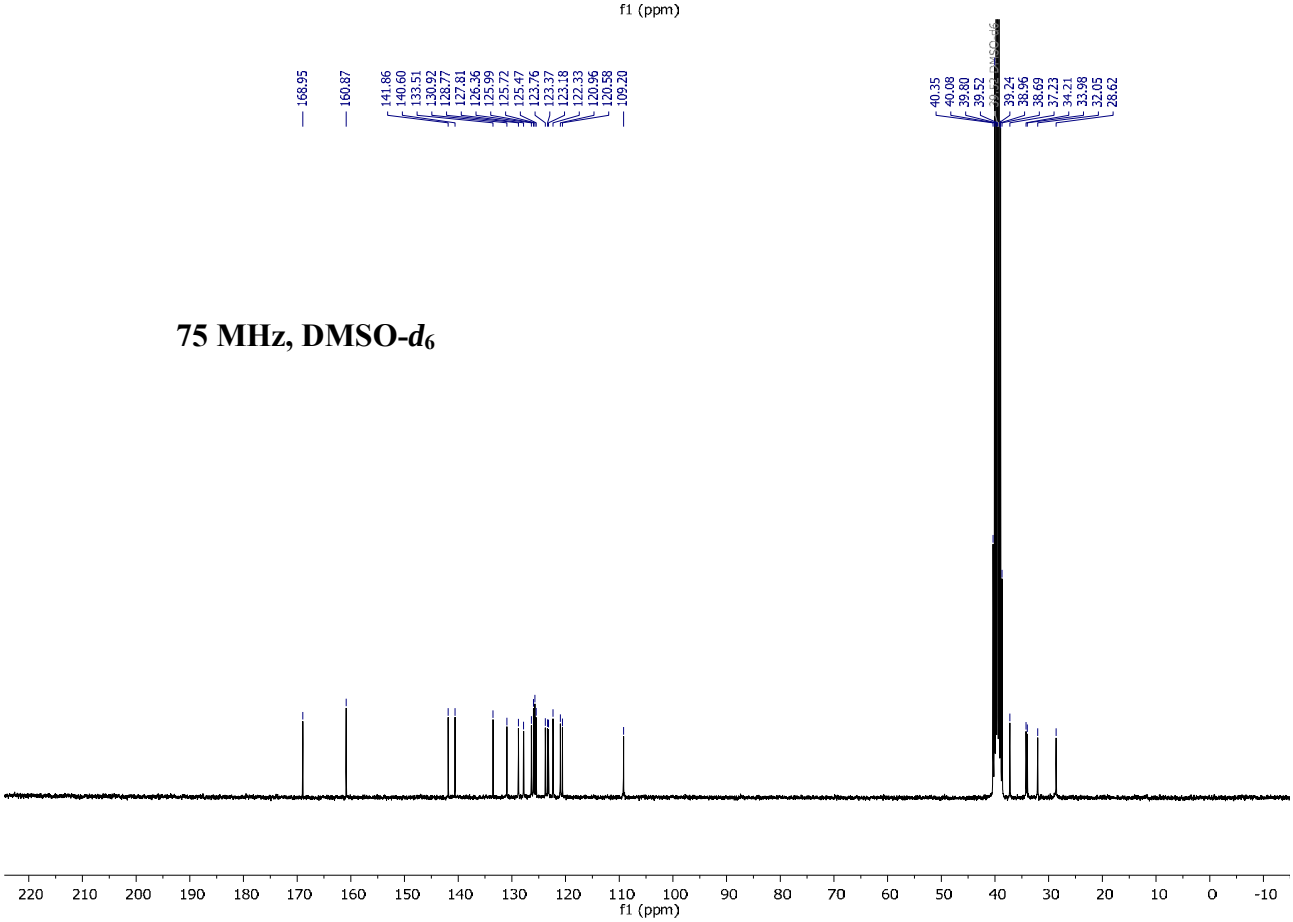
300 MHz, $CDCl_3$



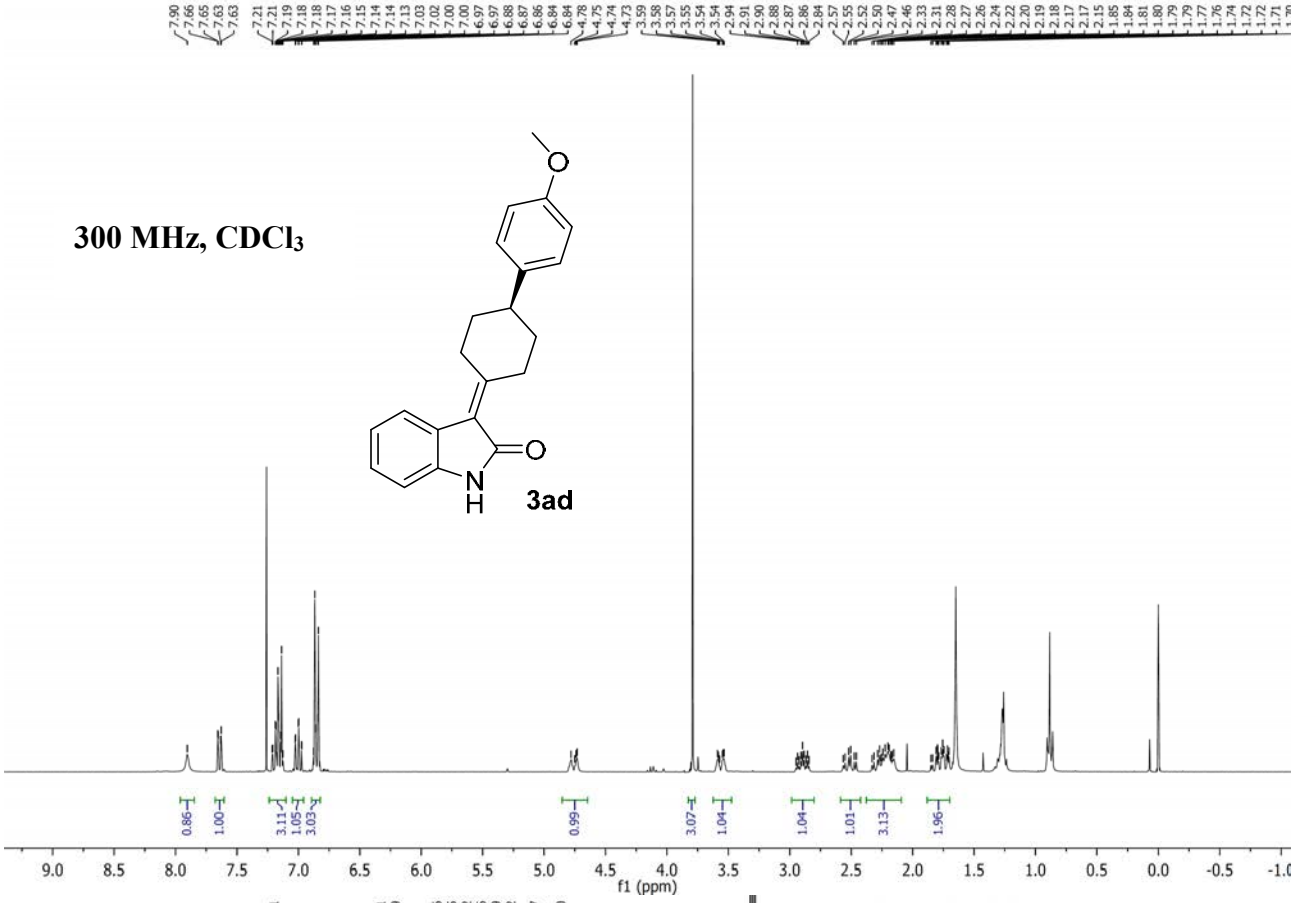
75 MHz, $CDCl_3$



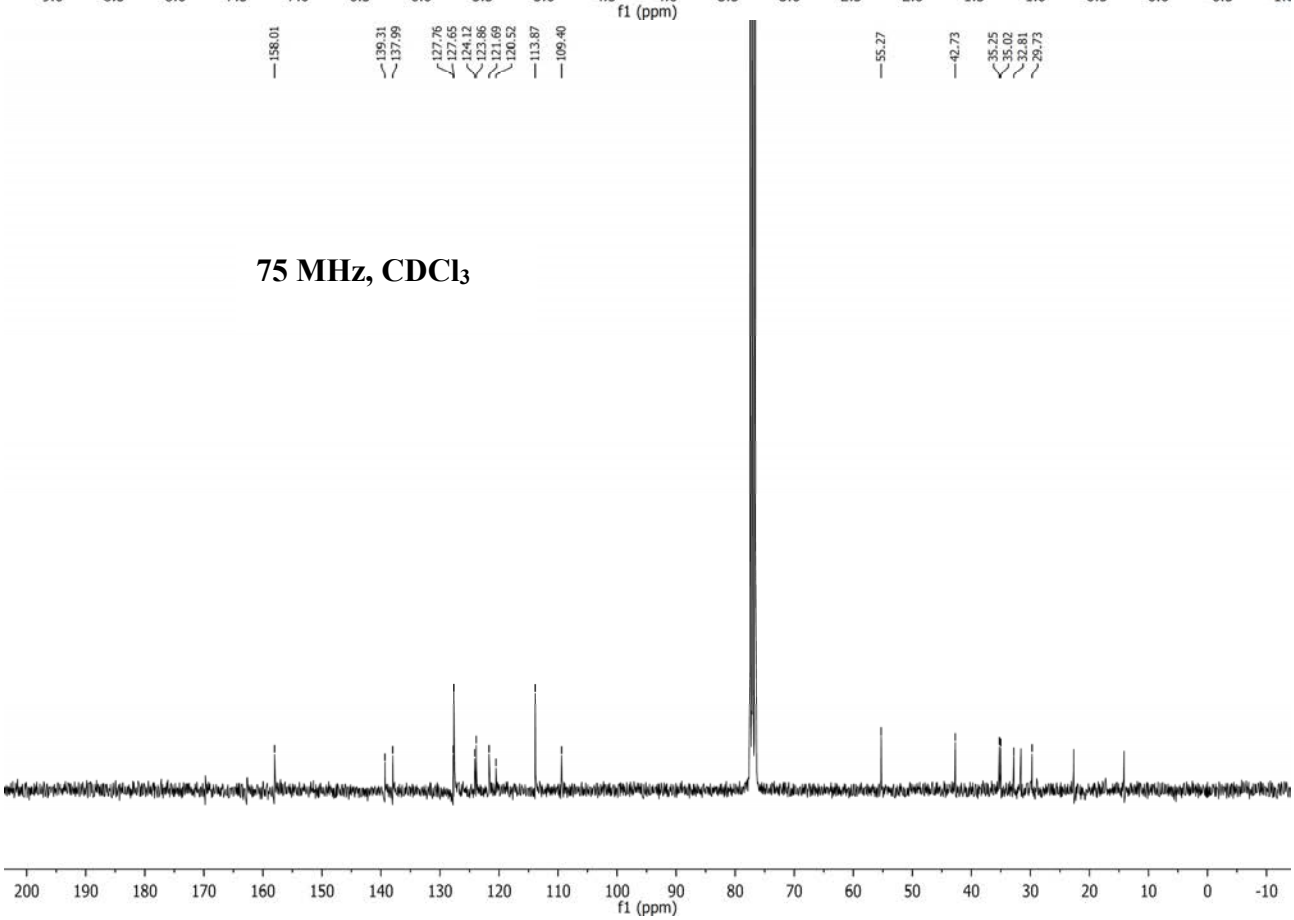

400 MHz, DMSO-d_6
3ac
f1 (ppm)

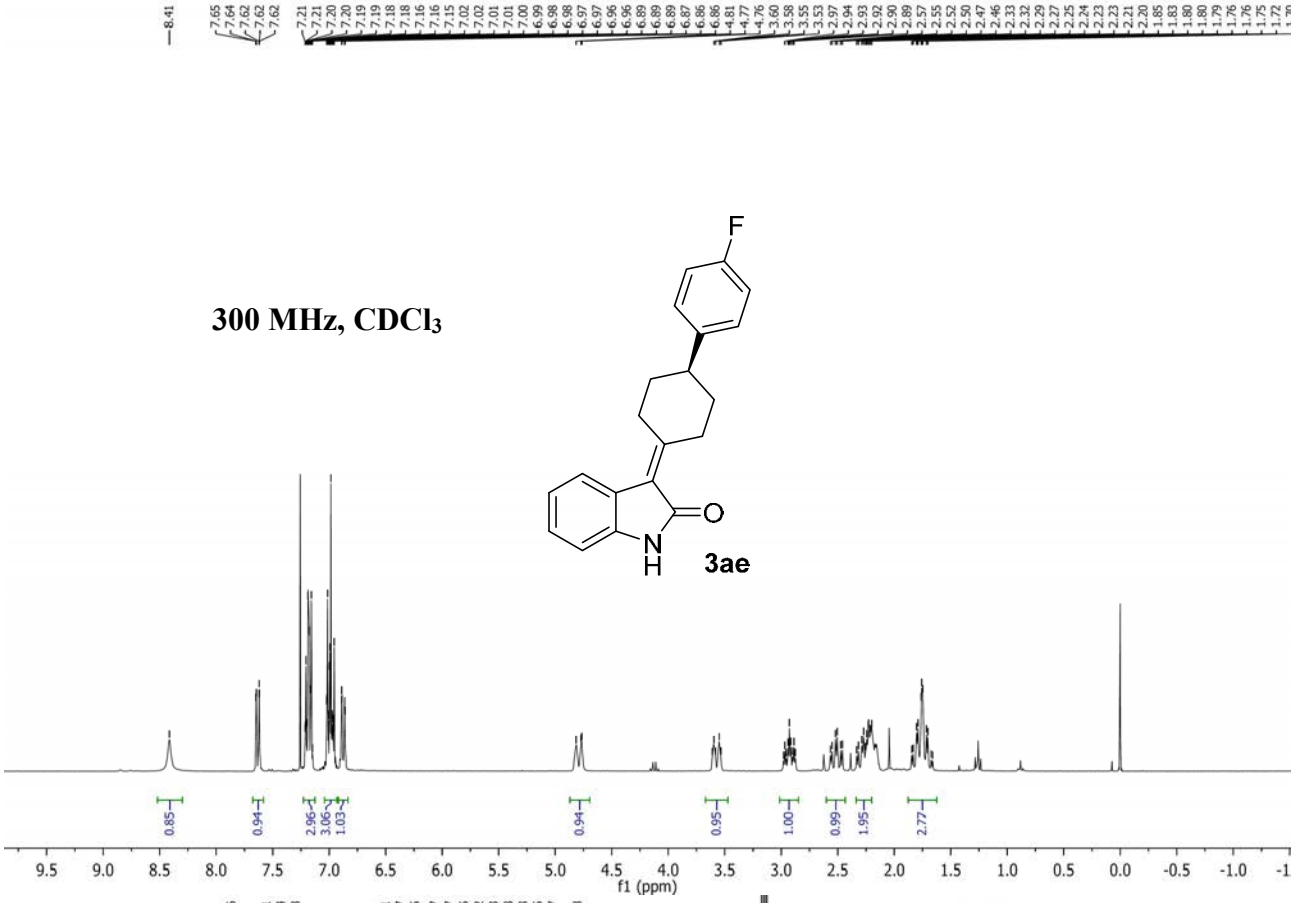

75 MHz, DMSO-d_6
f1 (ppm)

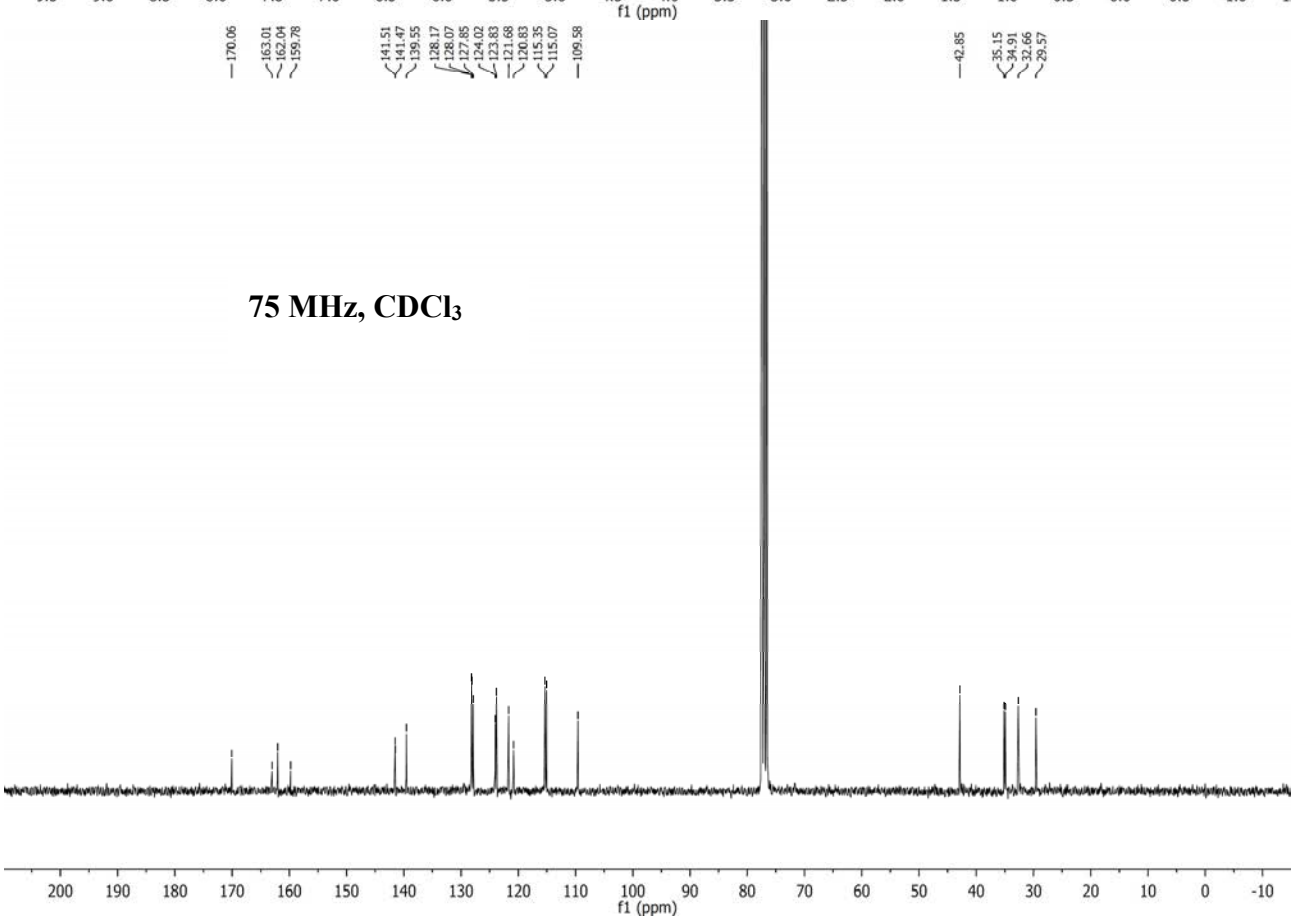
300 MHz, $CDCl_3$



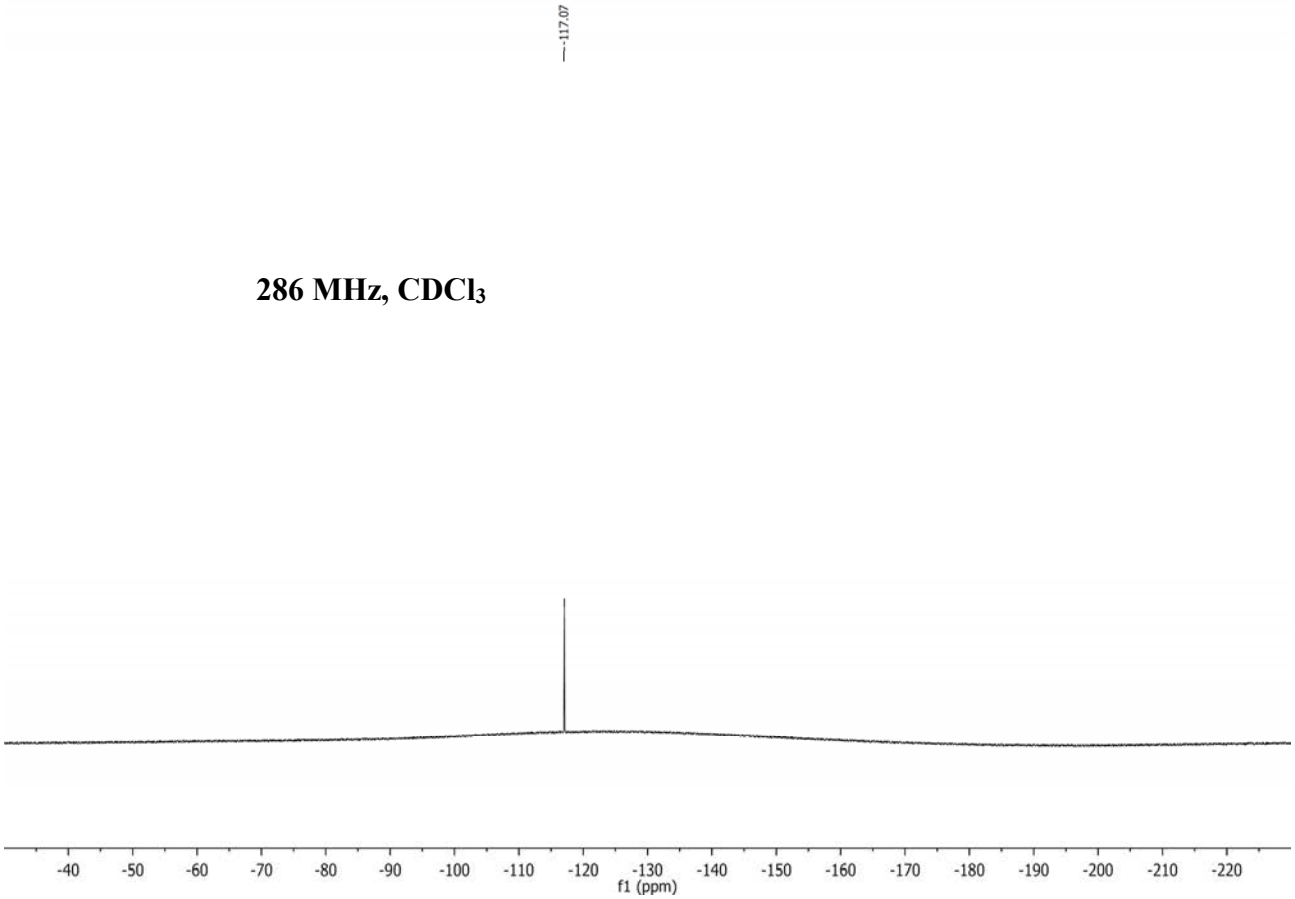
75 MHz, $CDCl_3$




300 MHz, CDCl3
F
O
N
H
3ae
f1 (ppm)

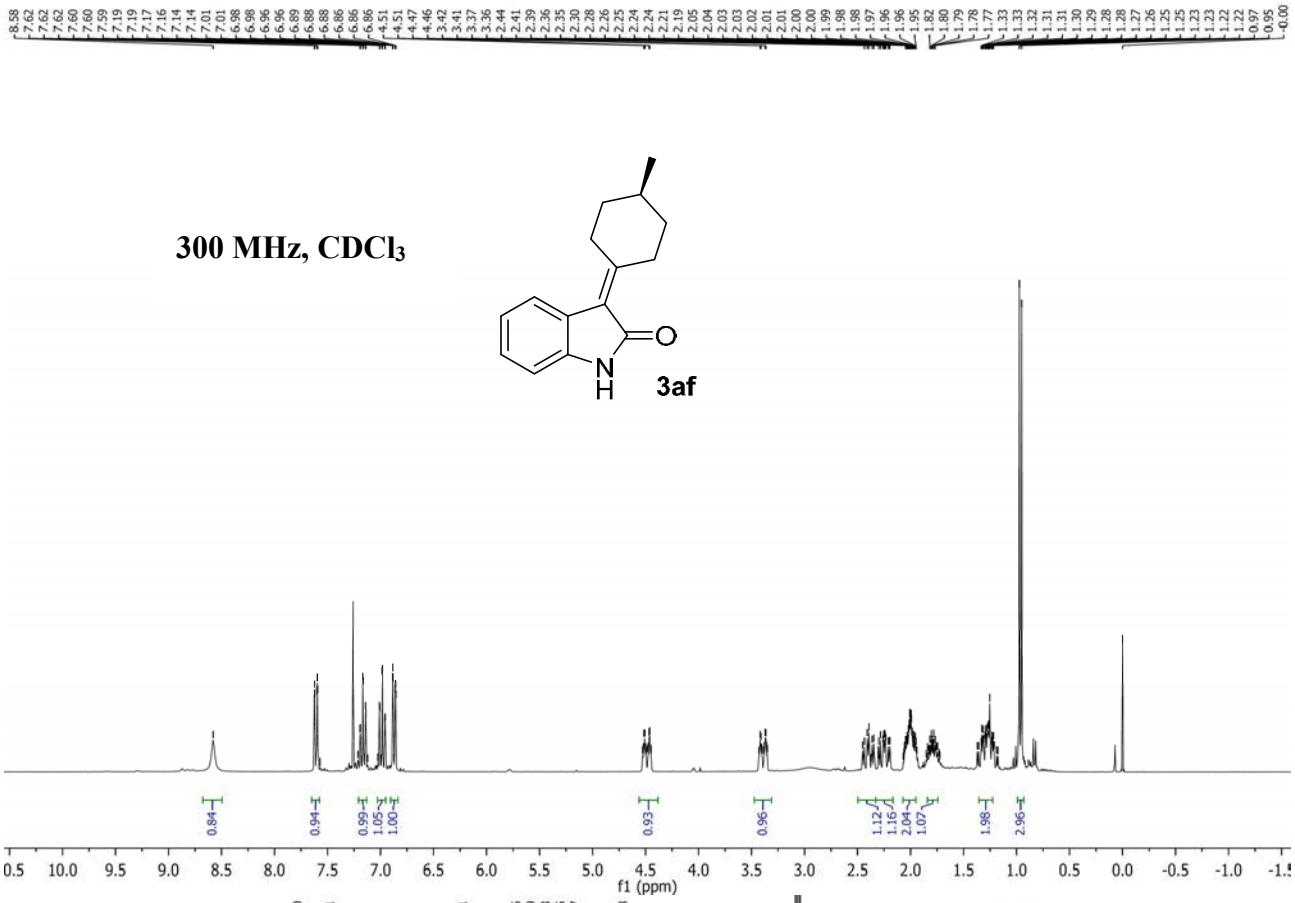

75 MHz, CDCl3
f1 (ppm)

286 MHz, $CDCl_3$

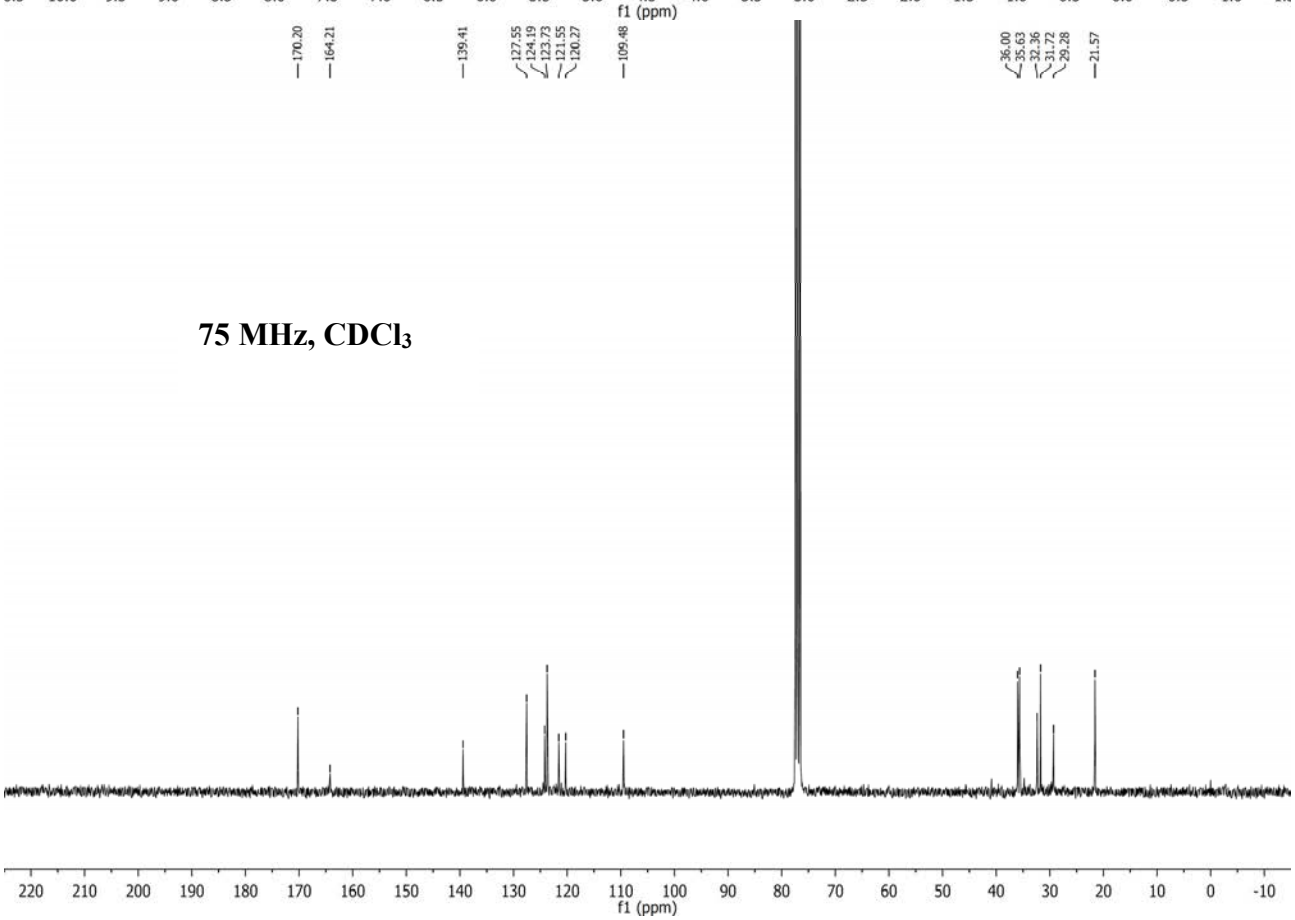


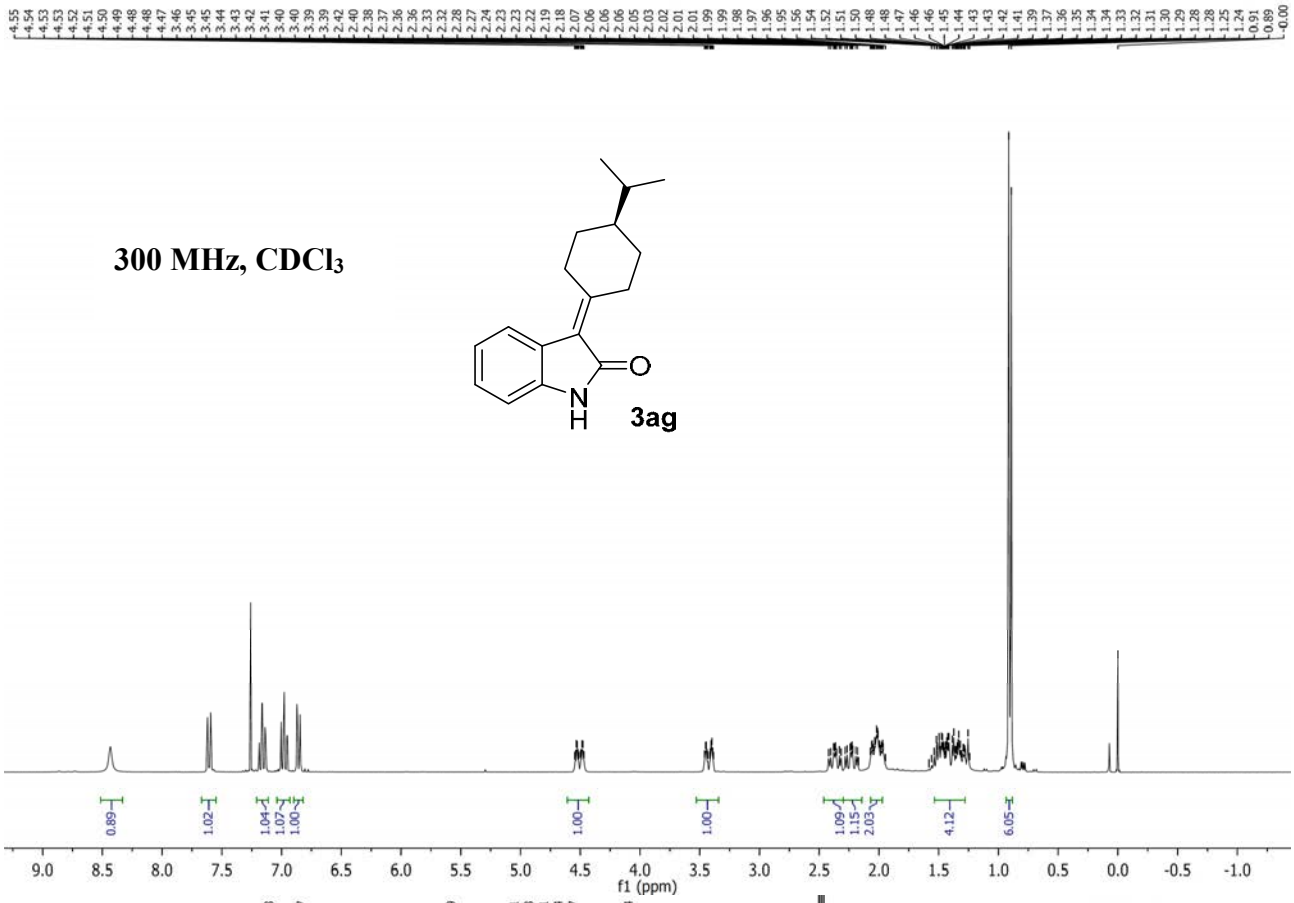
300 MHz, $CDCl_3$

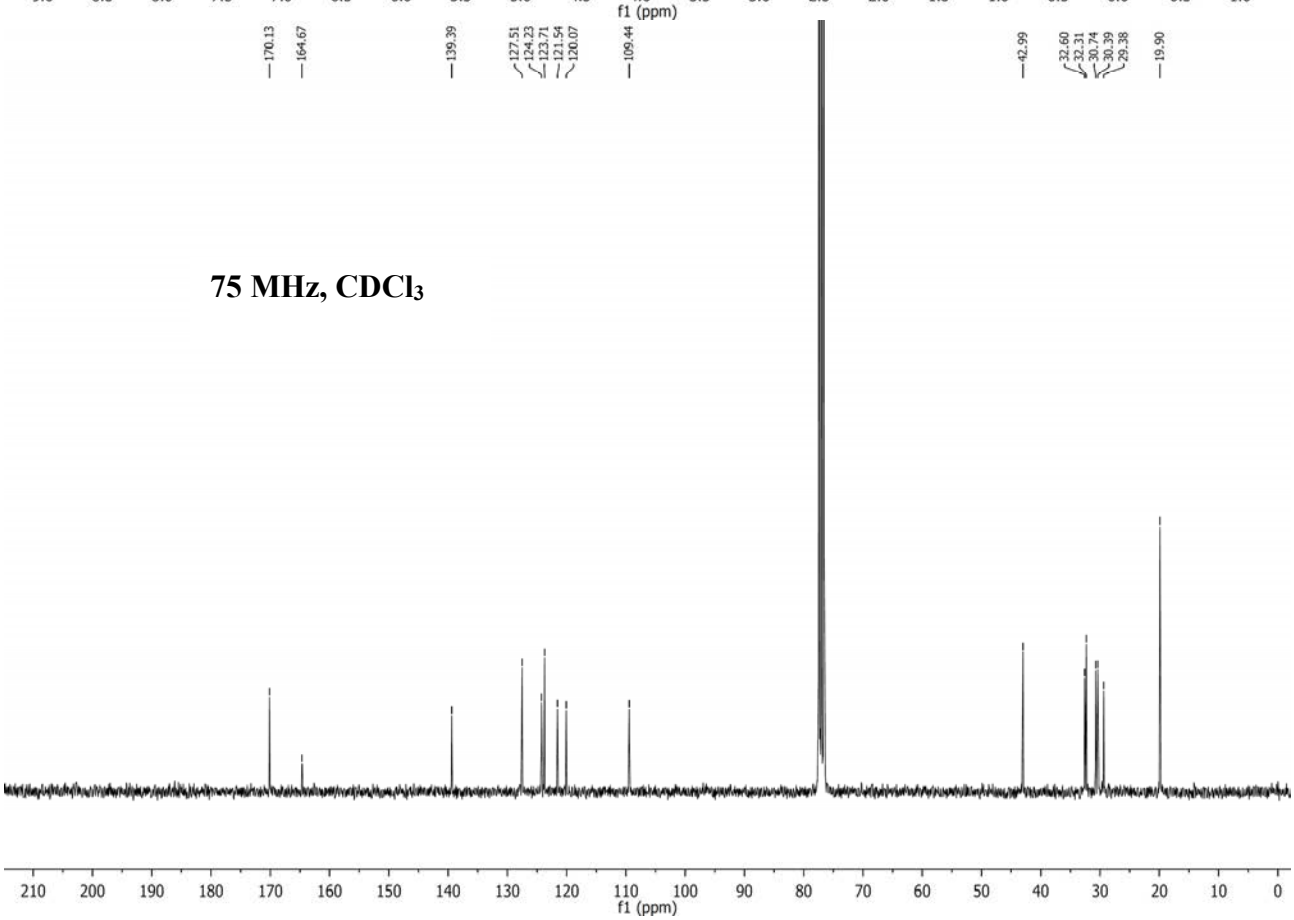
3af

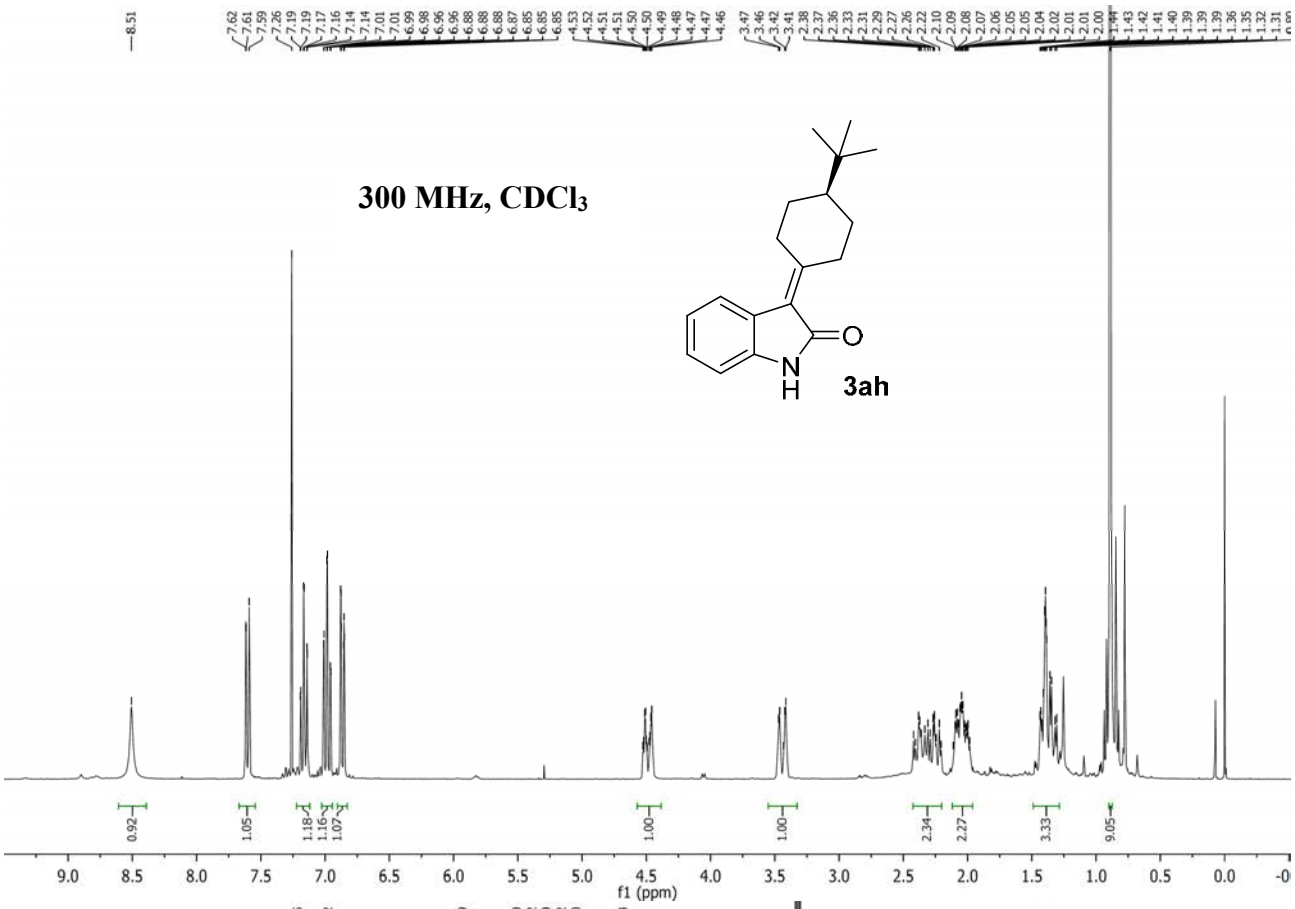


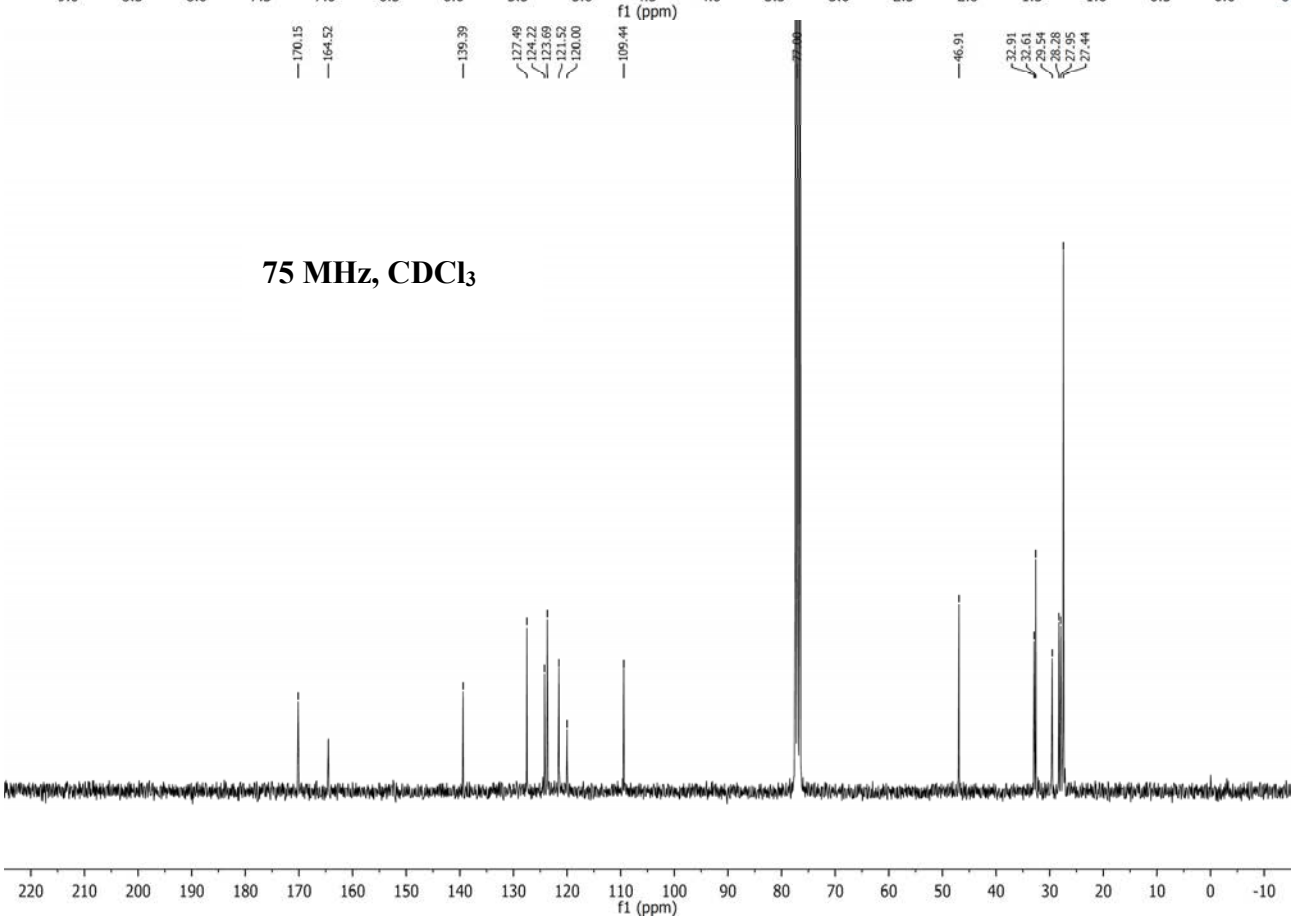
75 MHz, $CDCl_3$




300 MHz, CDCl3
3ag
f1 (ppm)

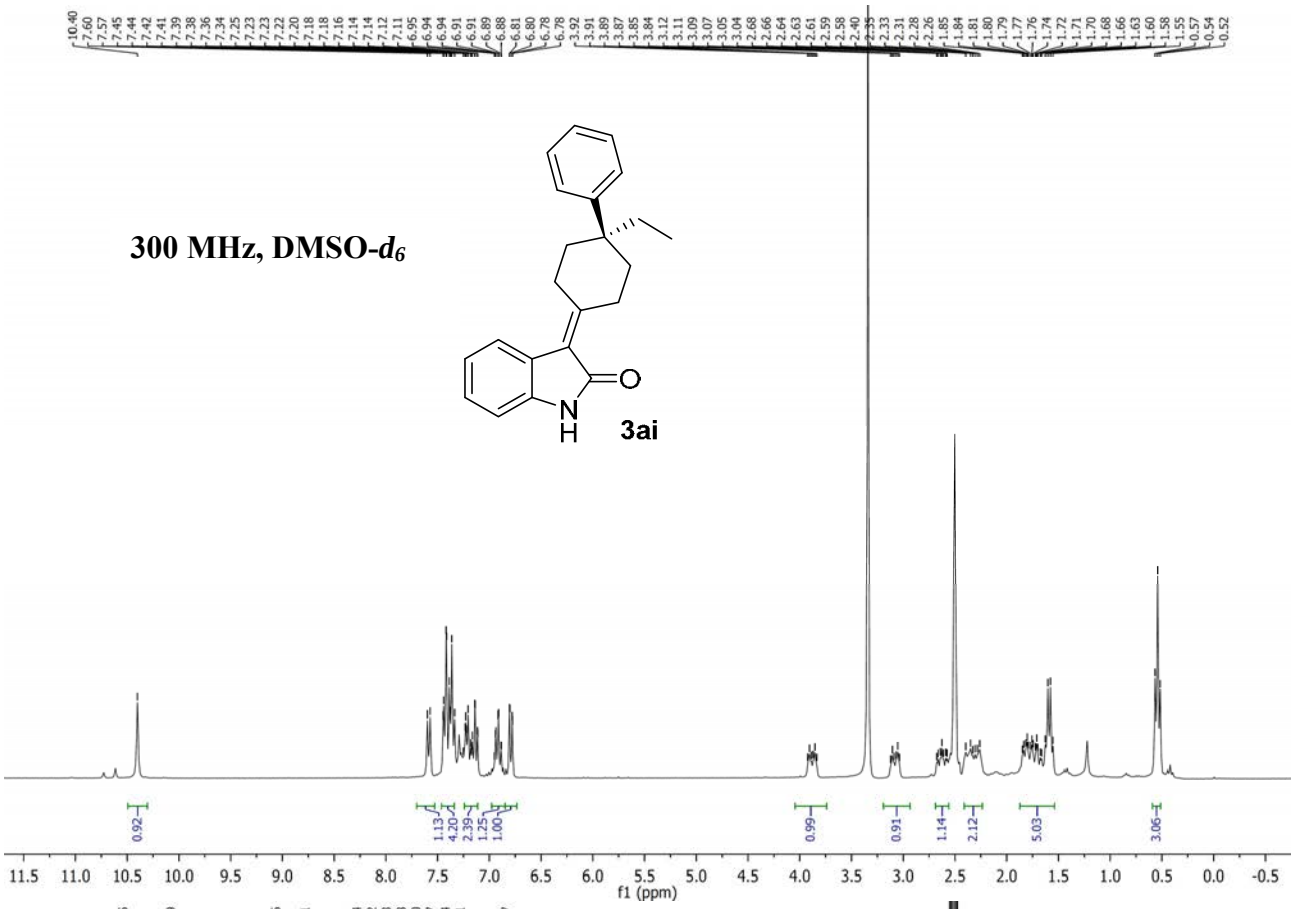

75 MHz, CDCl3
f1 (ppm)


300 MHz, CDCl3
3ah
f1 (ppm)

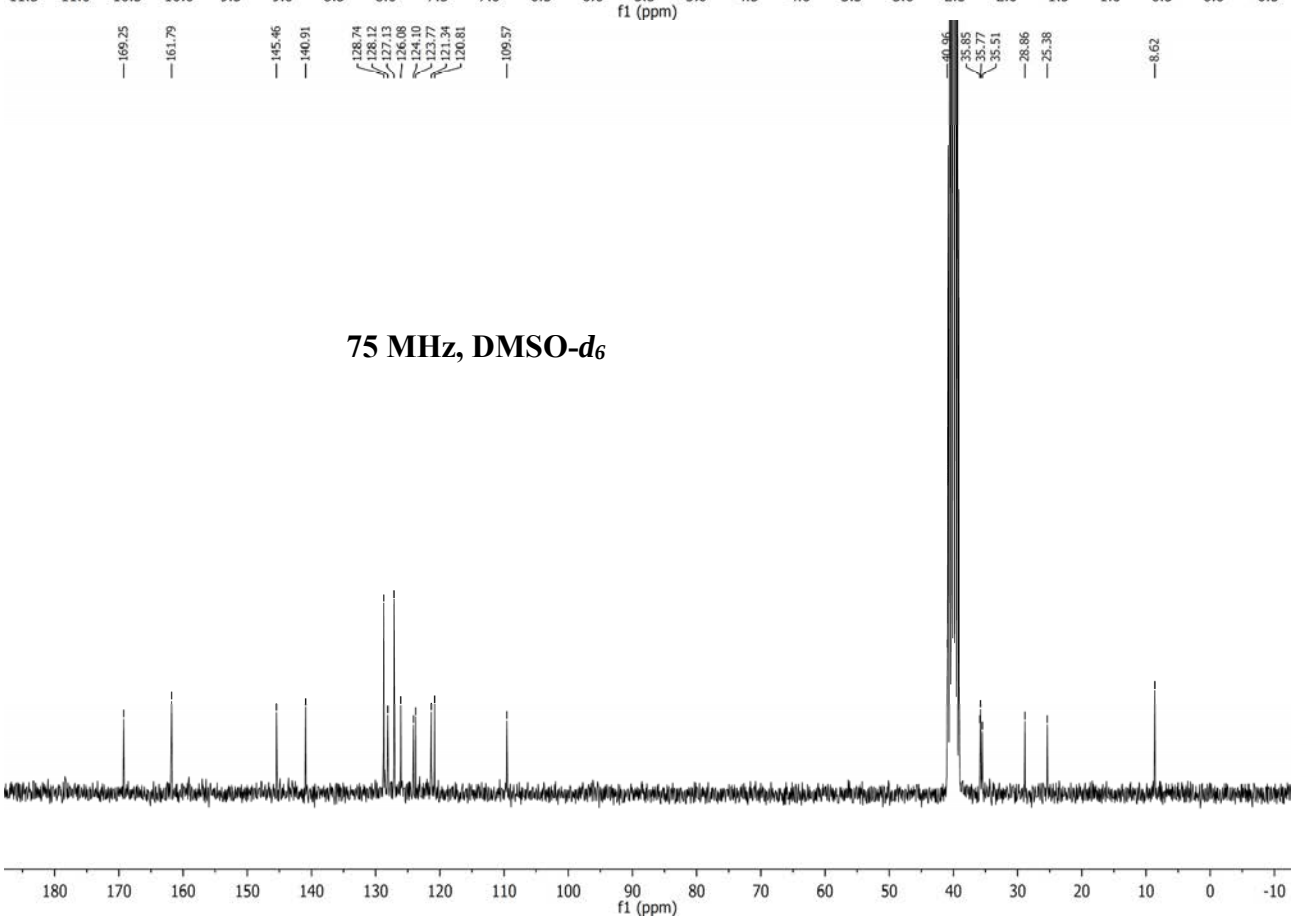

75 MHz, CDCl3
f1 (ppm)

300 MHz, DMSO-*d*6

3ai

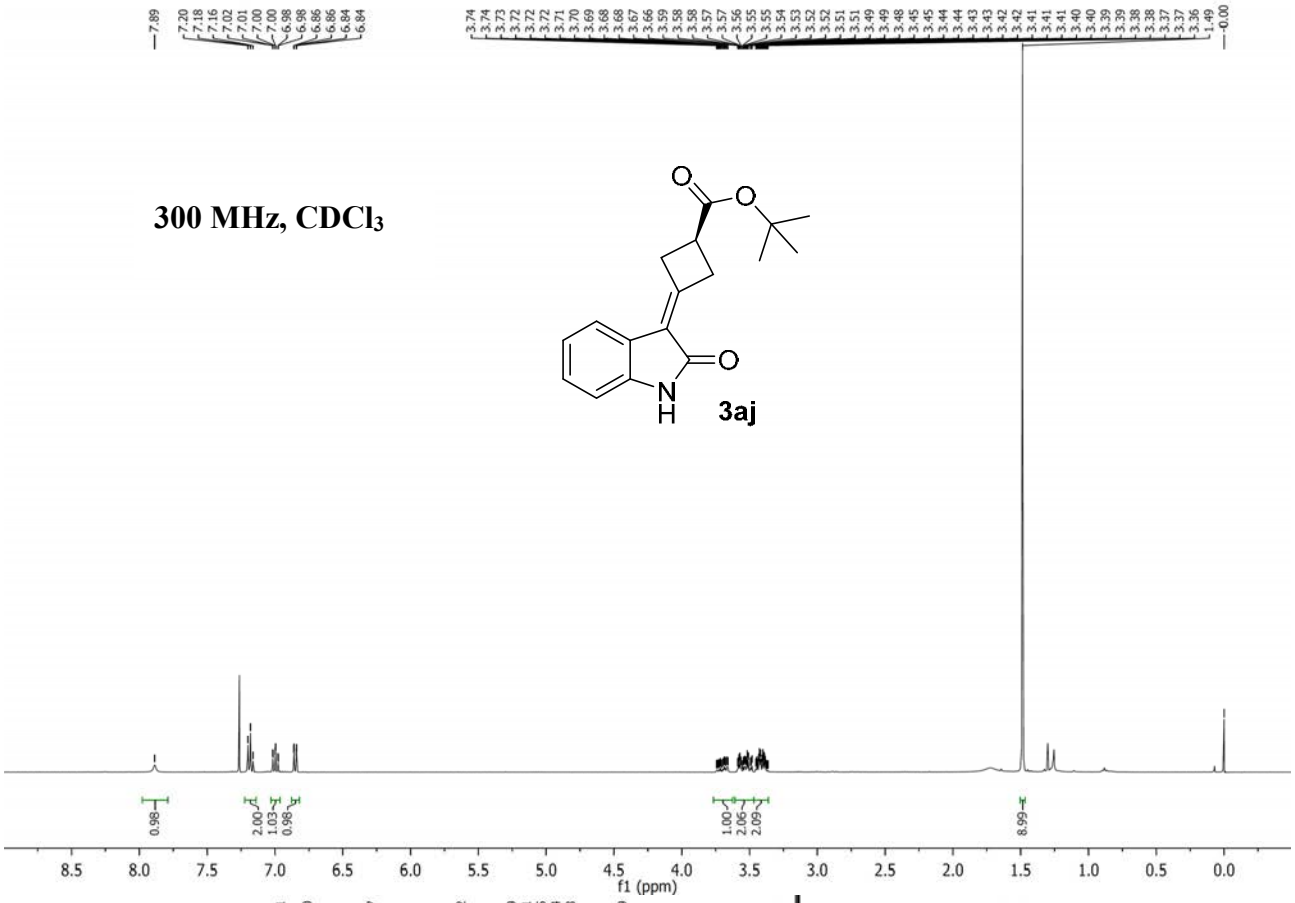


75 MHz, DMSO-*d*6

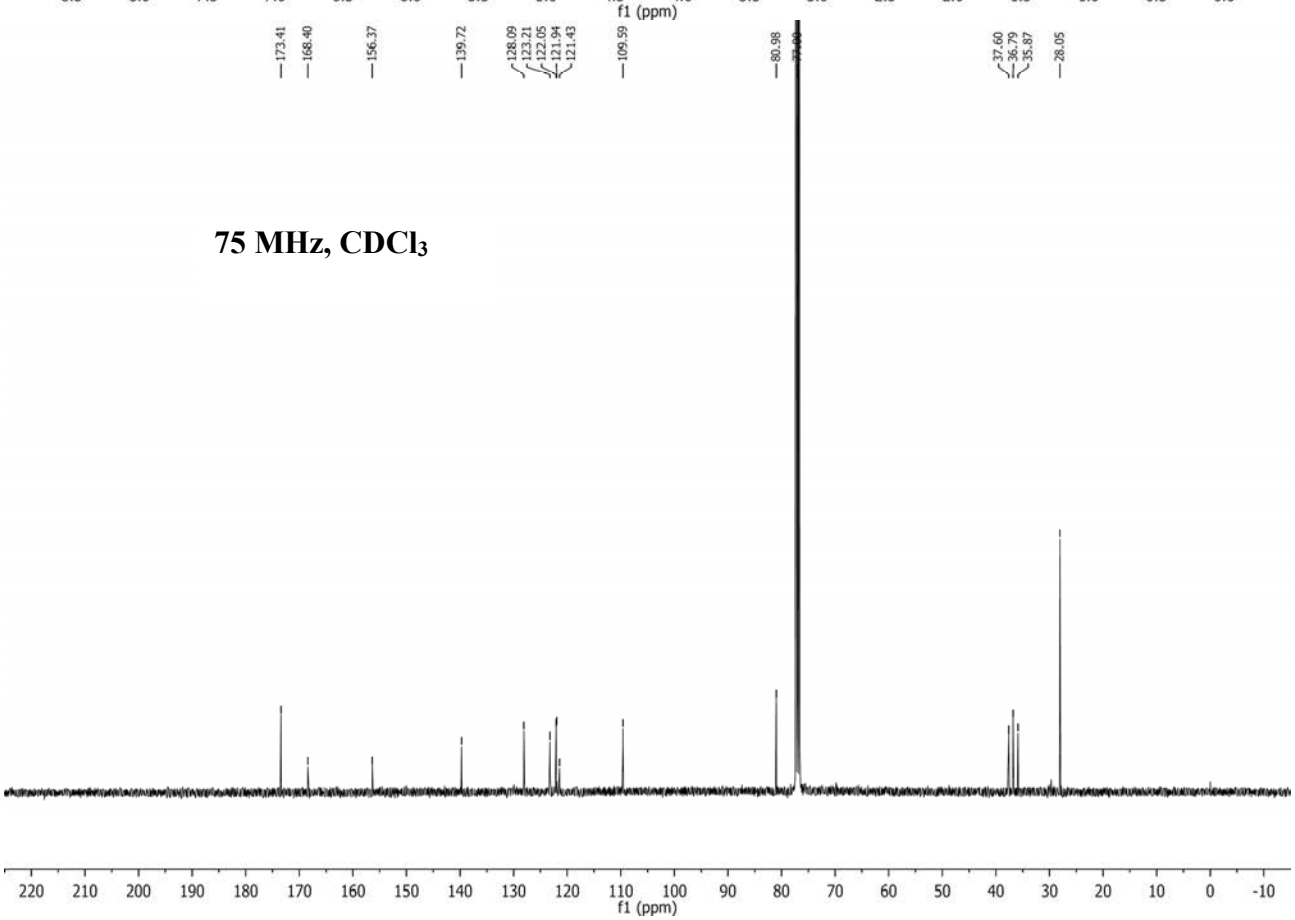


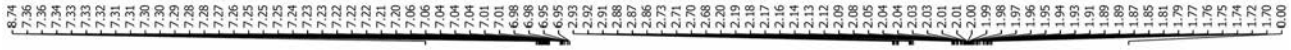
300 MHz, $CDCl_3$

3aj

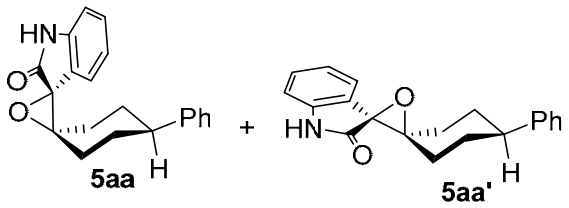


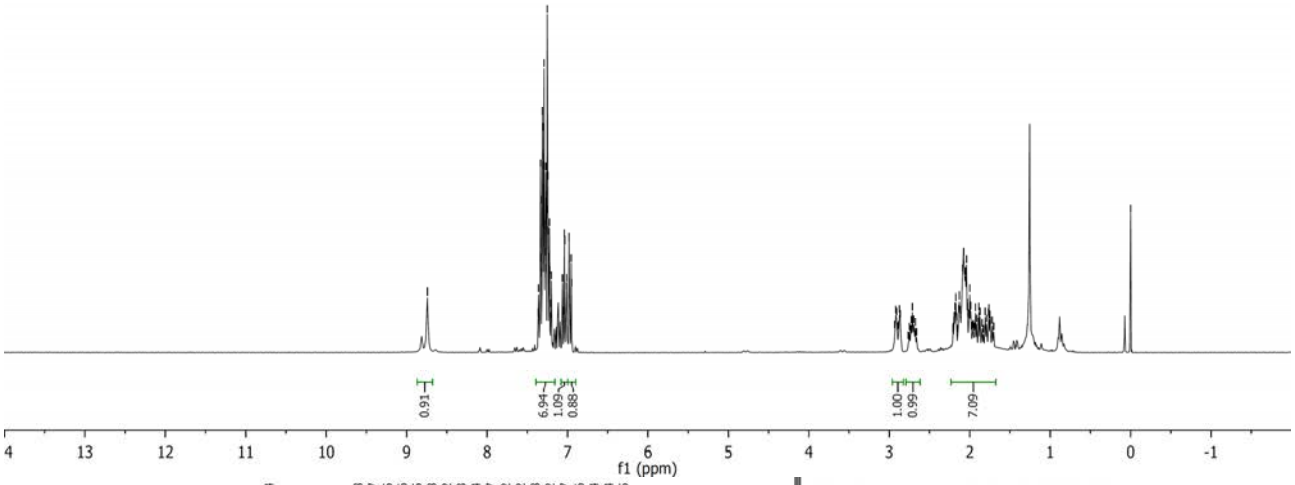
75 MHz, $CDCl_3$



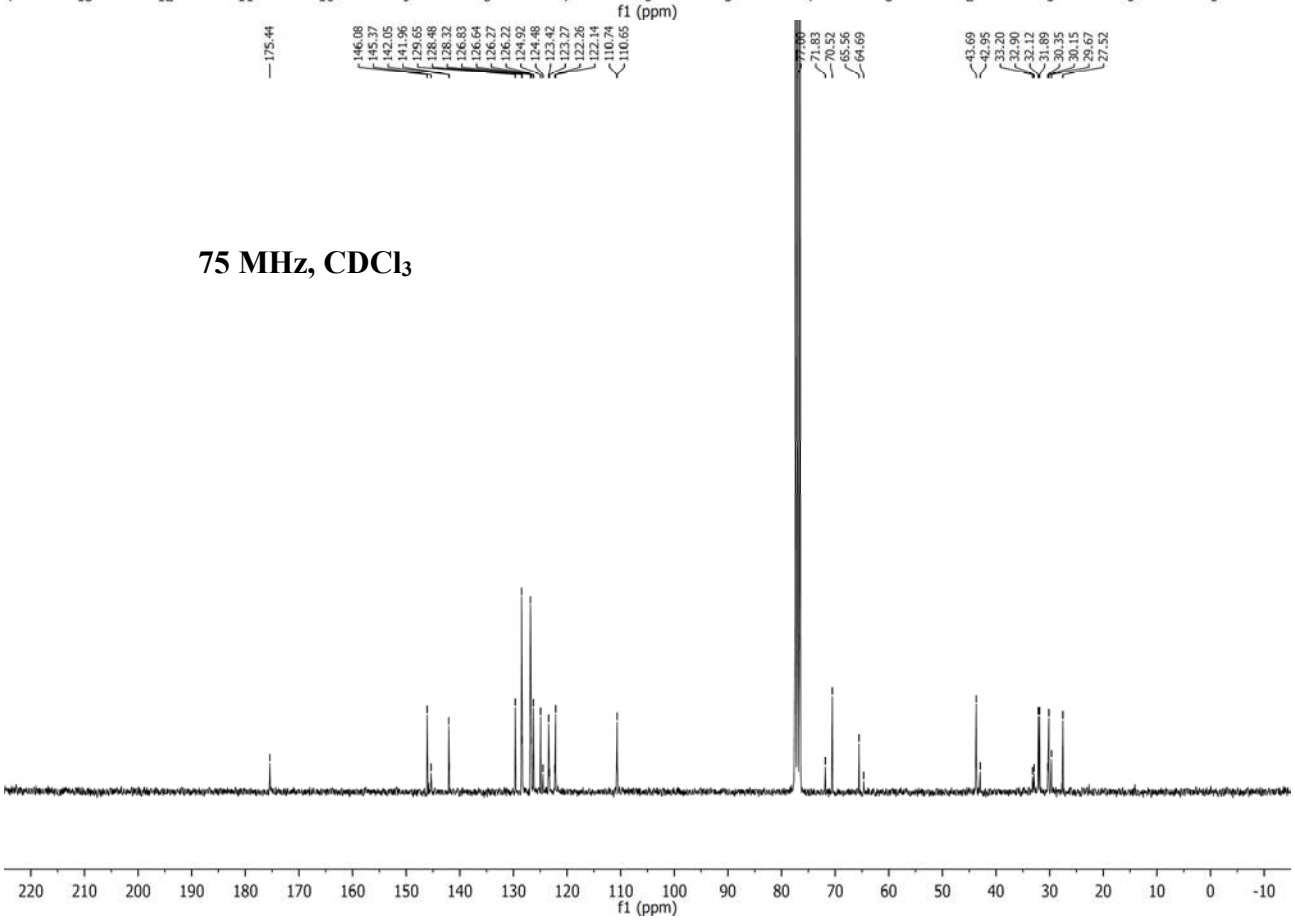


300 MHz, $CDCl_3$



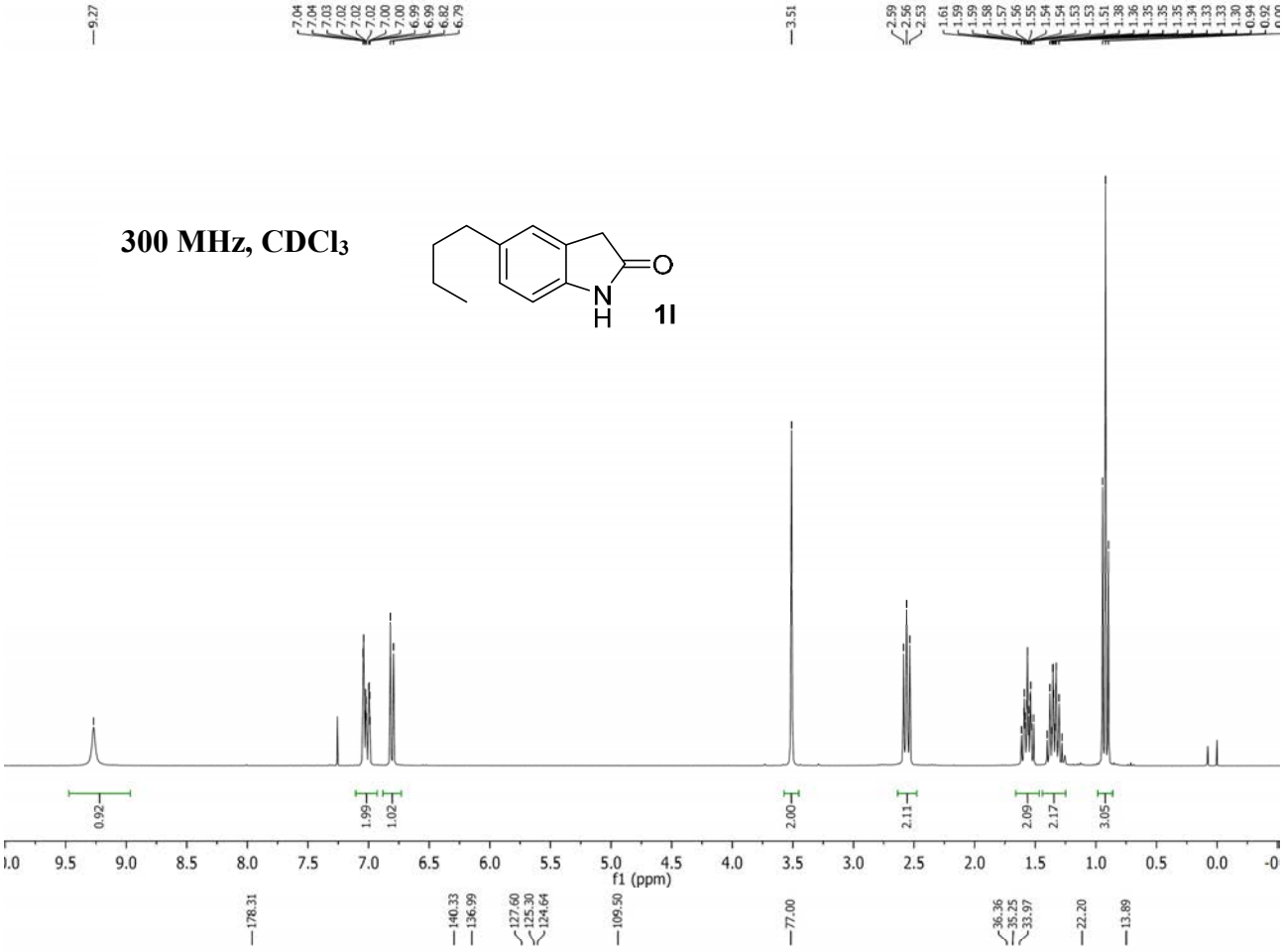


75 MHz, $CDCl_3$

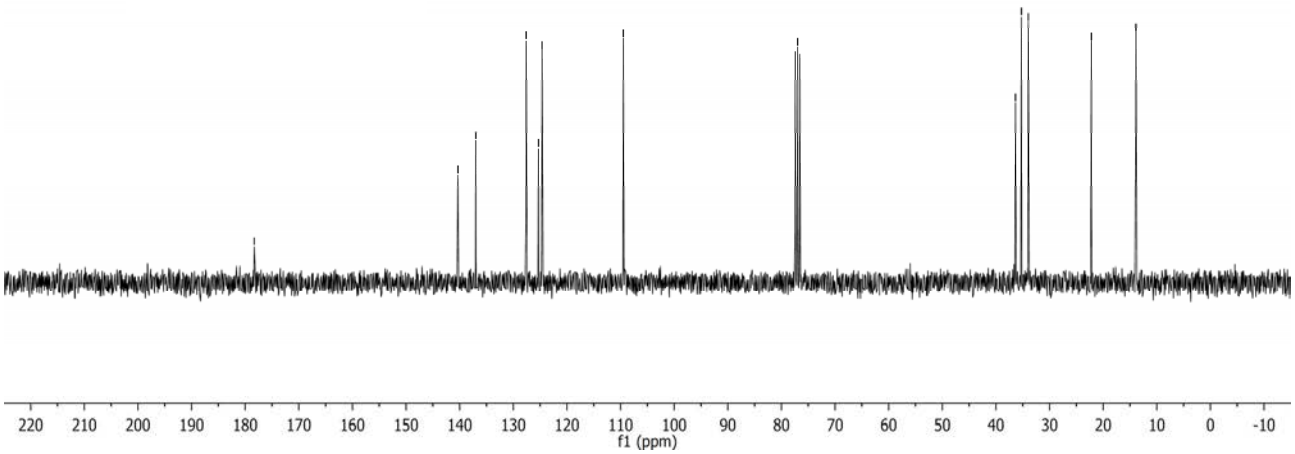


300 MHz, $CDCl_3$

1l



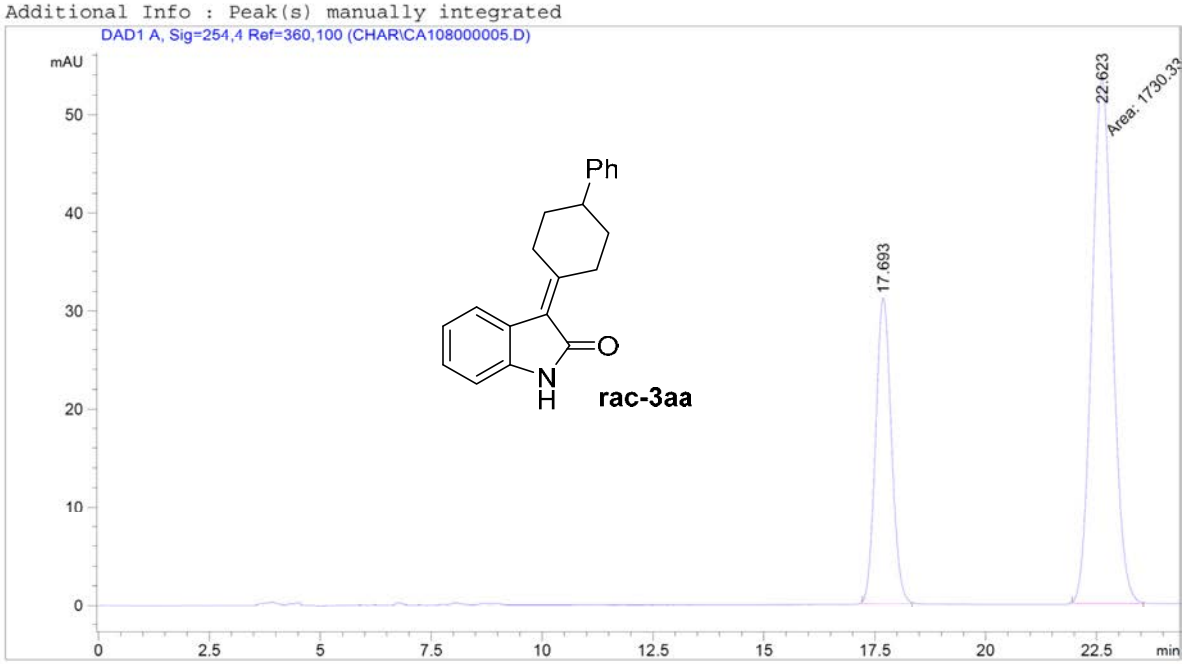
75 MHz, $CDCl_3$



HPLC TRACES

Data File C:\CHEM32\2\DATA\CHAR\CA108000005.D
Sample Name: CA_108_colonna_secco

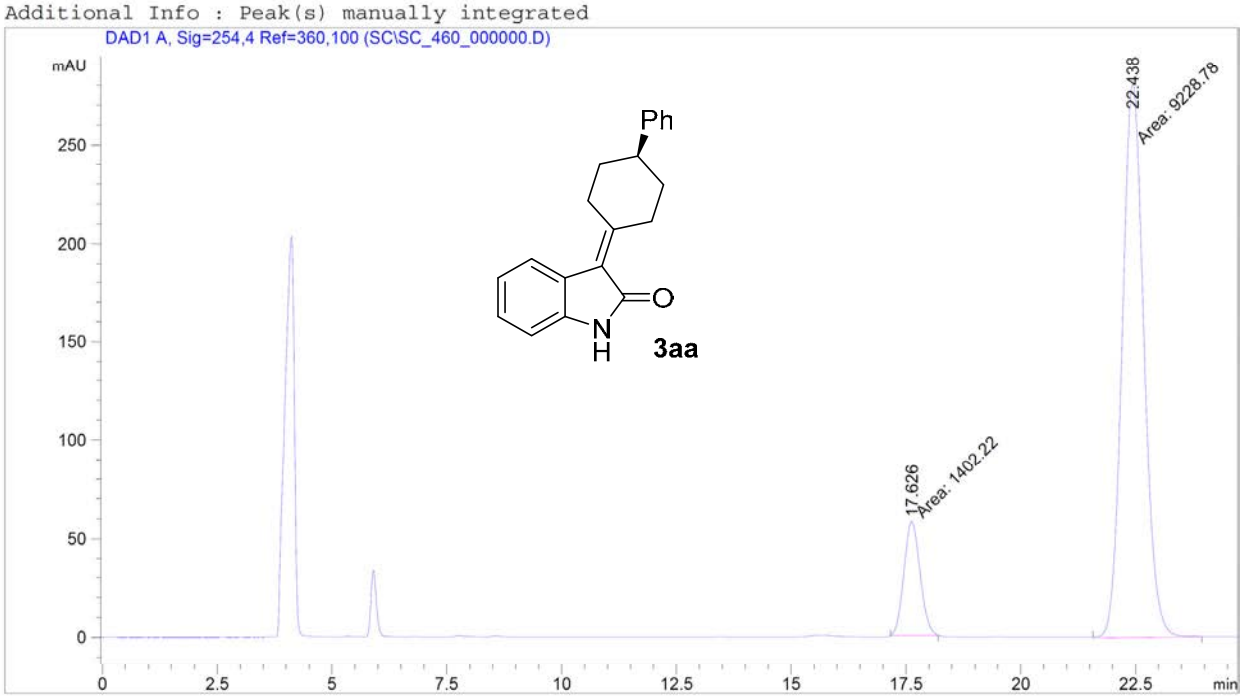
```
==================================================================
Acq. Operator   : chiara
Acq. Instrument : chiral                          Location : Vial 12
Injection Date  : 23/05/2018 17:39:59
                                                 Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\2\METHODS\TMP.M
Last changed    : 23/05/2018 17:33:02 by chiara
                  (modified after loading)
Analysis Method : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed    : 19/12/2018 12:35:41 by Davide
                  (modified after loading)
Sample Info     : CA_108_colonna_secco ; Hex/IPA 70/30; 0.8 mL/min; 25 gr
                  adi


Additional Info : Peak(s) manually integrated
```




```
==================================================================
                          Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.693 BB    0.3839  768.92712   31.15666  30.7662
   2  22.623 MM    0.5404 1730.32922   53.36865  69.2338

Totals :                  2499.25635   84.52531


chiral 19/12/2018 17:23:02 Davide                          Page   1 of 2
```

Data File C:\CHEM32\2\DATA\SC\SC_460_000000.D
Sample Name: SC_460

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 60
Injection Date   : 11/10/2018 11:52:33
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 11/10/2018 11:51:00 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 19/12/2018 12:35:41 by Davide
                   (modified after loading)
Sample Info      : SC_460; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

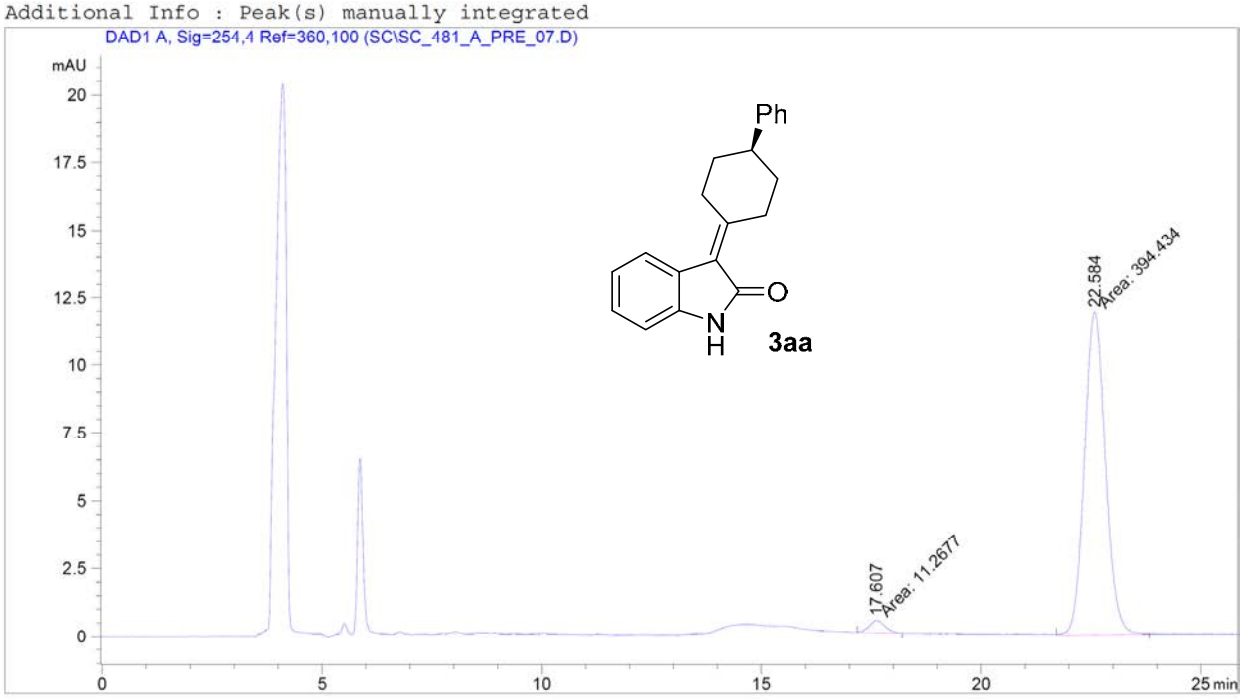



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  17.626 MM    0.4062 1402.22302   57.53912  13.1899
   2  22.438 MM    0.5475 9228.77734  280.92395  86.8101

Totals :                  1.06310e4   338.46307


==================================================================
```

chiral 19/12/2018 17:15:00 Davide Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_481_A_PRE_07.D
Sample Name: SC_481_A_pre

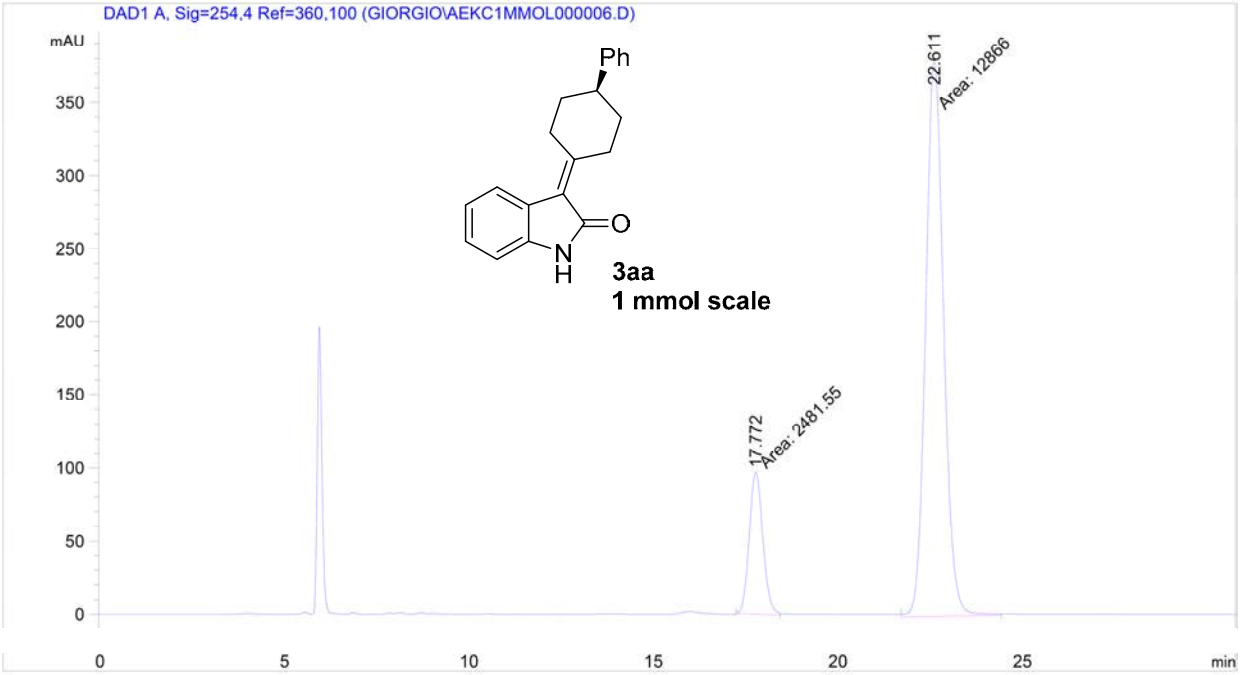
```
==========================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 1
Injection Date   : 08/11/2018 16:00:21
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 08/11/2018 14:55:51 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 19/12/2018 12:35:41 by Davide
                   (modified after loading)
Sample Info      : SC_481_A_pre; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
                   ;


Additional Info : Peak(s) manually integrated
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  17.607 MM    0.4142   11.26770 4.53386e-1   2.7773
   2  22.584 MM    0.5519  394.43399   11.91051  97.2227

Totals :                   405.70170   12.36389
```

Data File C:\CHEM32\2\DATA\GIORGIO\AEKC1MMOL000006.D
Sample Name: aEKC1mmol

```
==================================================================
Acq. Operator    : giorgio
Acq. Instrument  : chiral                          Location : Vial 41
Injection Date   : 28/02/2019 11:20:25
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\LAB_COM_18.M
Last changed     : 28/02/2019 11:05:51 by Michele
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\LAB_COM_18.M
Last changed     : 07/03/2019 15:07:29 by giorgio
                   (modified after loading)
Sample Info      : aEKC1mmol, ADH 70:30, 0.8 ml/min,


Additional Info : Peak(s) manually integrated
```

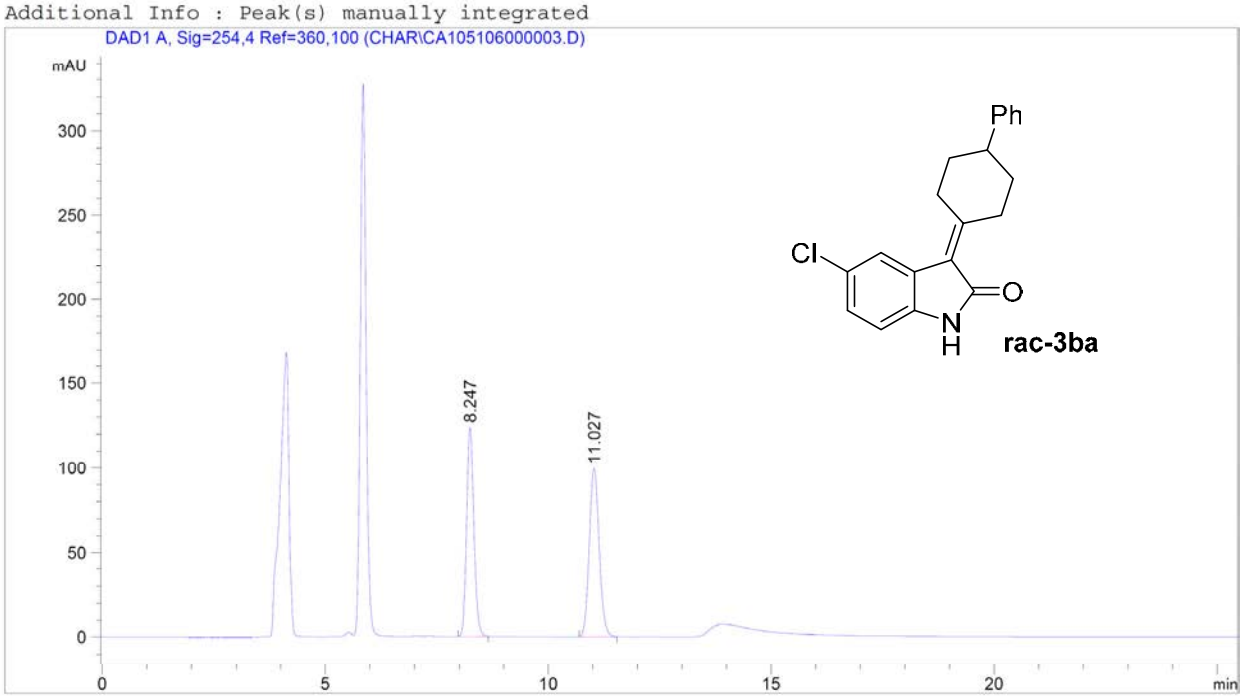



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.772 MM    0.4265 2481.55200   96.97914  16.1690
   2  22.611 MM    0.5635 1.28660e4   380.56848  83.8310

Totals :                  1.53476e4   477.54762


==================================================================
```

chiral 07/03/2019 15:09:39 giorgio Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA105106000003.D
Sample Name: CA_Cloxindole_racemo

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 11
Injection Date   : 18/05/2018 10:06:12
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 18/05/2018 09:52:15 by stefano
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : CA_Cloxindole_racemo; Hex/IPA 70/30; 0.8 mL/min; 25 gra
                   di

Additional Info : Peak(s) manually integrated
```



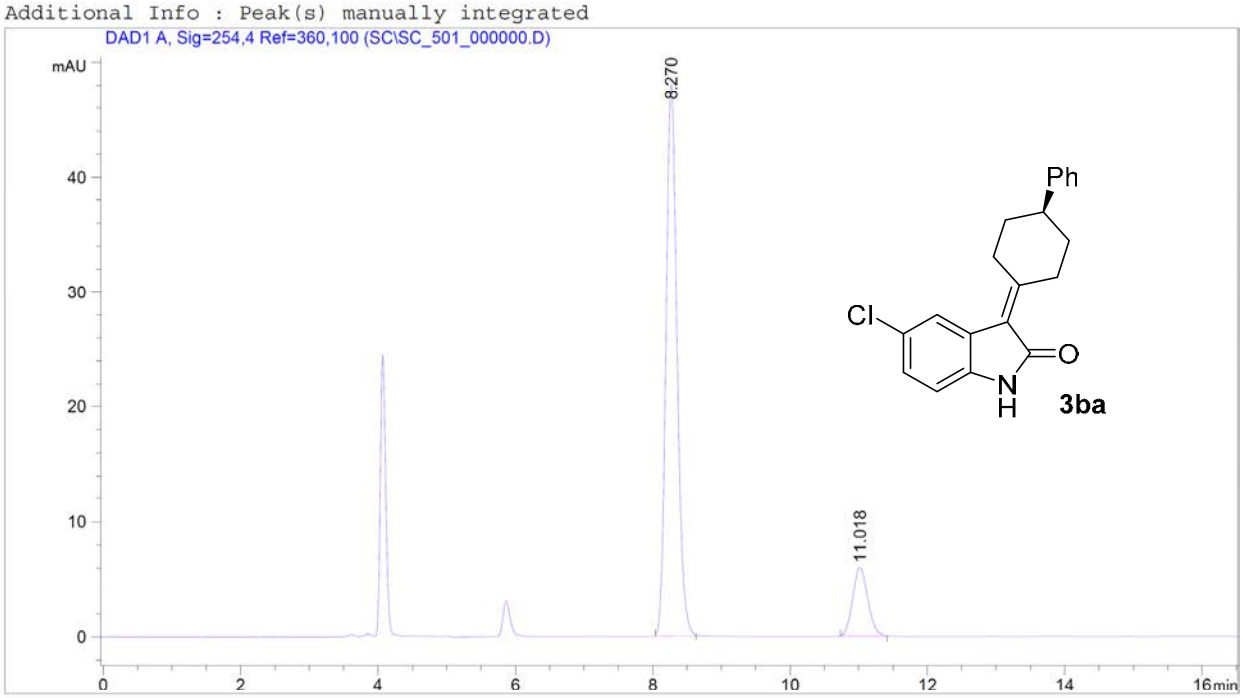

```
==================================================================
                          Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.247 BB    0.1745 1405.63623  123.74204  47.7439
   2  11.027 BB    0.2384 1538.48059   99.50905  52.2561

Totals :                  2944.11682  223.25109


==================================================================
```

chiral 10/07/2018 11:26:45 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_501_000000.D
Sample Name: SC_501

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 1
Injection Date   : 30/11/2018 15:04:23
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 30/11/2018 14:54:31 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_501; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C
```

Additional Info : Peak(s) manually integrated



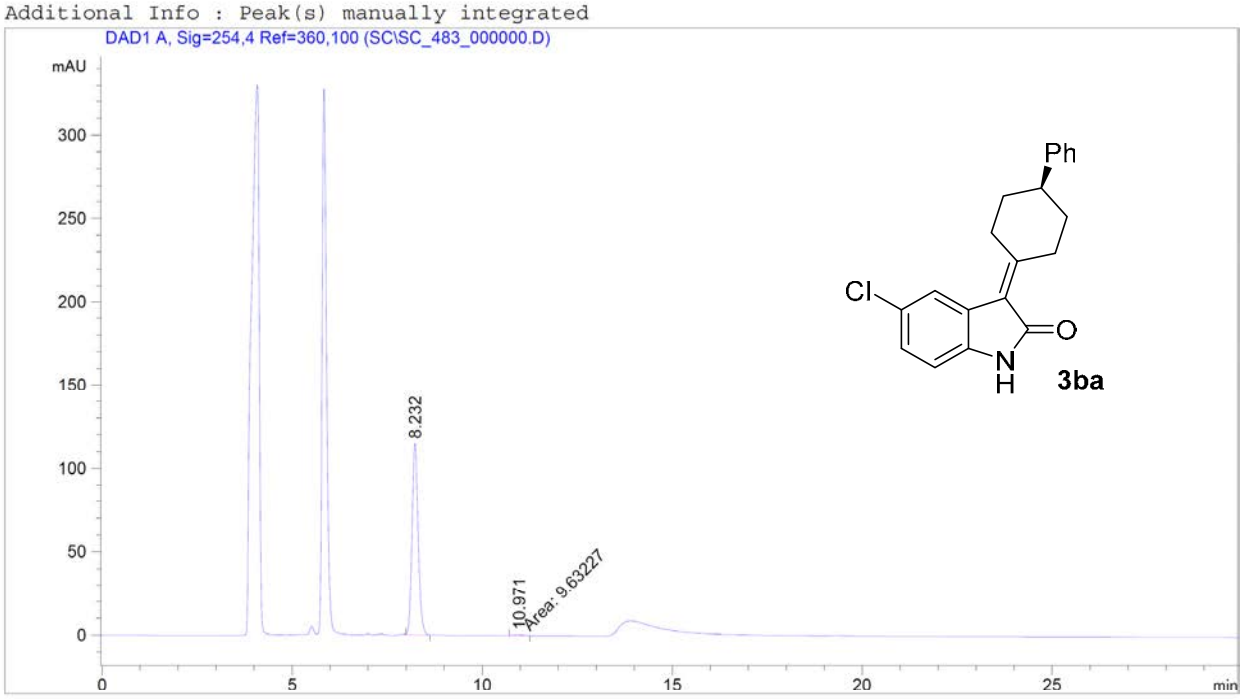

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.270 BB    0.1723  536.36609   48.03216  85.3618
   2  11.018 BB    0.2359   91.97865    6.03307  14.6382

Totals :                   628.34474   54.06523


==================================================================
                         *** End of Report ***
```

chiral 12/12/2018 11:25:42 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_483_000000.D
Sample Name: SC_483

```
==================================================================
Acq. Operator    : SIMONE
Acq. Instrument  : chiral                          Location : Vial 2
Injection Date   : 14/11/2018 10:29:32
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 14/11/2018 10:27:02 by SIMONE
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_483; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated



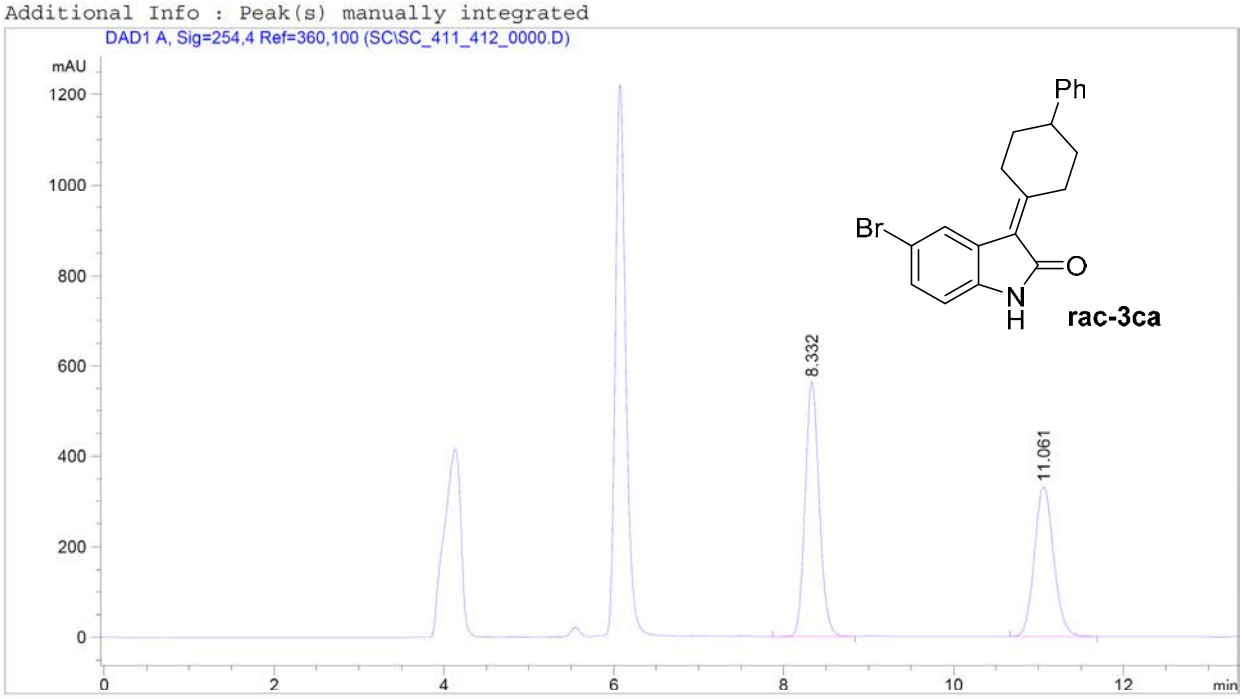

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.232 BB    0.1736 1293.30823  114.66847  99.2607
   2  10.971 MM    0.2242    9.63227 7.16196e-1   0.7393

Totals :                  1302.94050  115.38467


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 11:27:25 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_411_412_0000.D
Sample Name: SC_411_412

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 13
Injection Date   : 01/06/2018 16:58:32
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 01/06/2018 16:56:41 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : SC_411_412; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



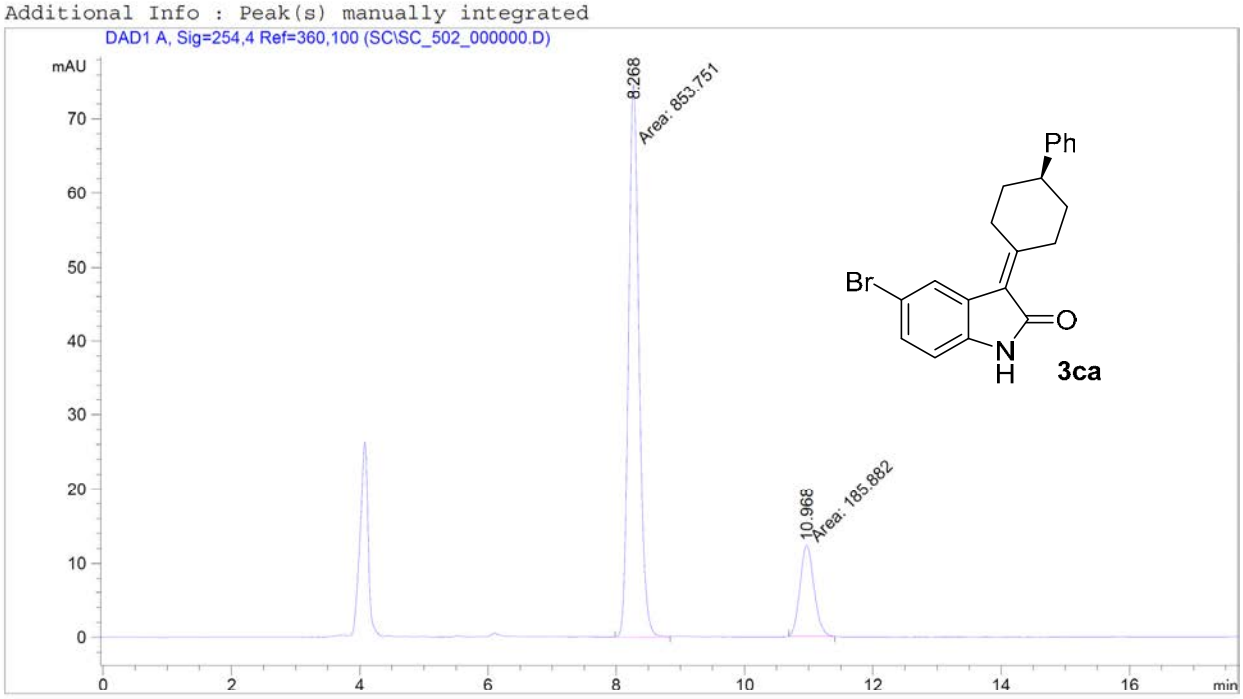

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.332 VB    0.1770 6529.78955  564.10168  55.5102
   2  11.061 BB    0.2438 5233.43652  332.19501  44.4898

Totals :                  1.17632e4   896.29669


==================================================================
                        *** End of Report ***
```

chiral 13/07/2018 14:44:47 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_502_000000.D
Sample Name: SC_502

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 2
Injection Date   : 30/11/2018 15:23:29
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 30/11/2018 15:21:19 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_502; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C
```

Additional Info : Peak(s) manually integrated

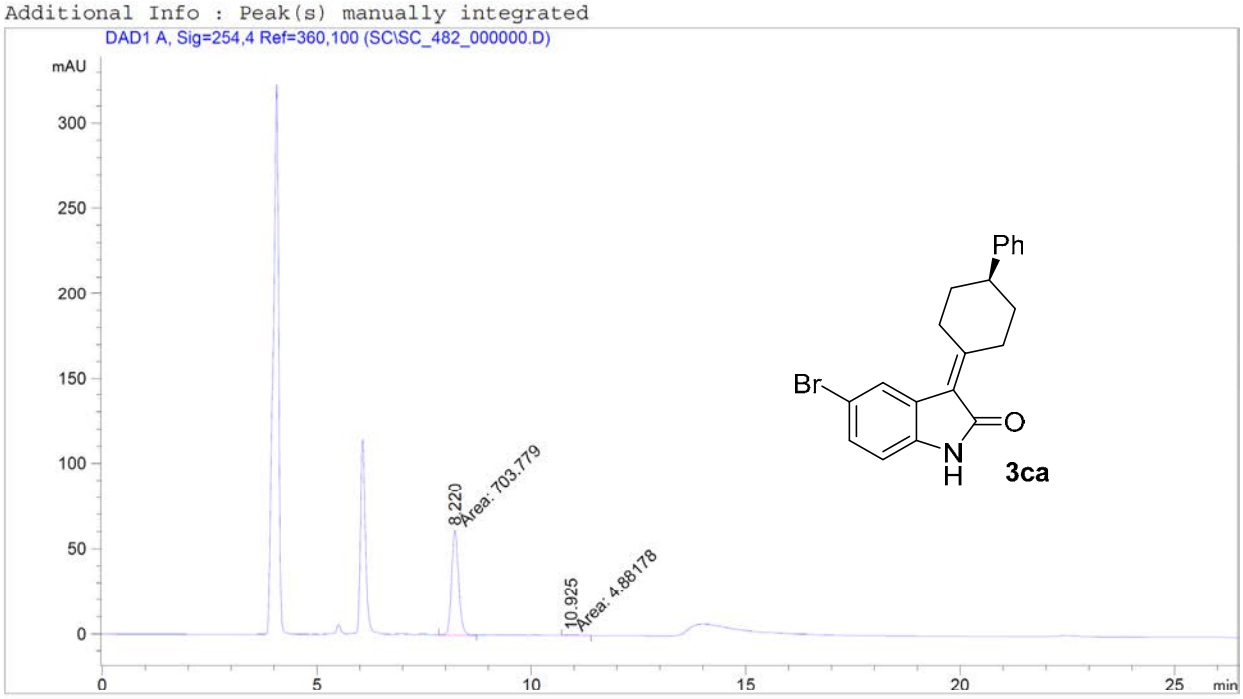



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.268 MM    0.1905  853.75146   74.70217  82.1204
   2  10.968 MM    0.2527  185.88235   12.25989  17.8796

Totals :                  1039.63382   86.96206


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 11:21:33 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_482_000000.D
Sample Name: SC_482

```
==================================================================
Acq. Operator    : SIMONE
Acq. Instrument  : chiral                          Location : Vial 1
Injection Date   : 14/11/2018 10:00:10
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 14/11/2018 09:58:00 by SIMONE
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_482; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

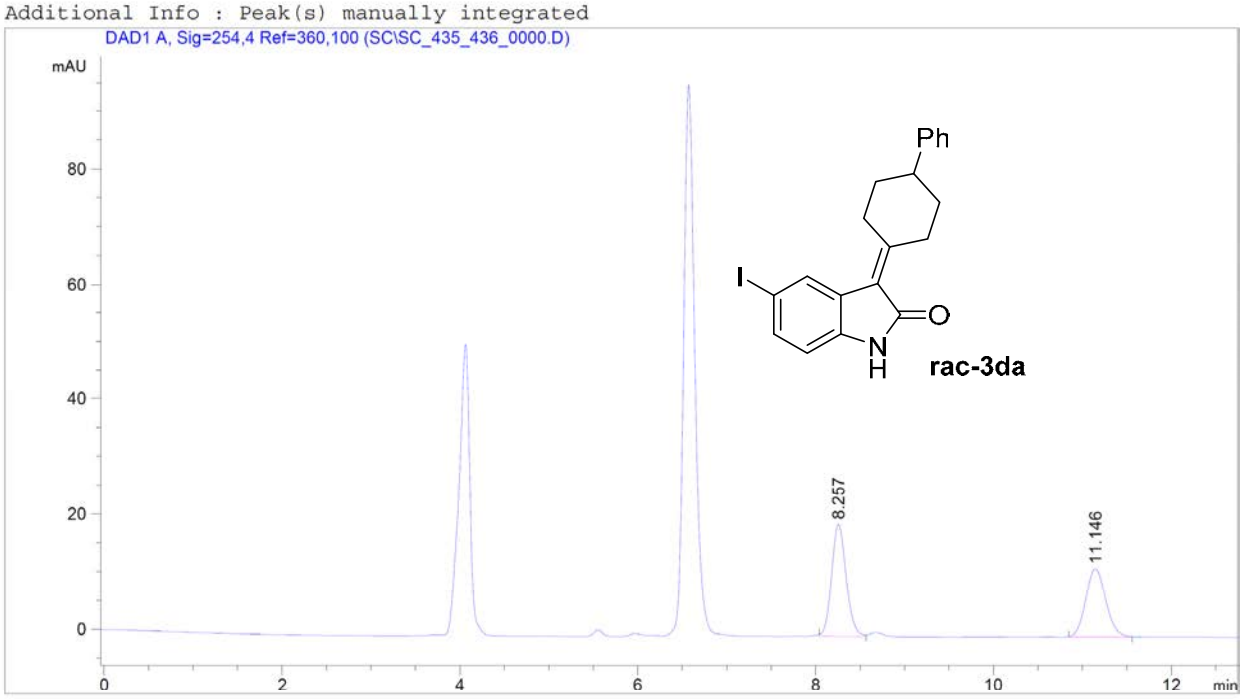



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.220 MM    0.1908  703.77899   61.48651  99.3111
   2  10.925 MM    0.2311    4.88178 3.52140e-1   0.6889

Totals :                   708.66077   61.83865


==================================================================
                         *** End of Report ***
```

chiral 12/12/2018 11:18:55 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_435_436_0000.D
Sample Name: SC_435_436

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 34
Injection Date   : 18/07/2018 10:28:04
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 18/07/2018 09:58:38 by stefano
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : SC_435_436; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

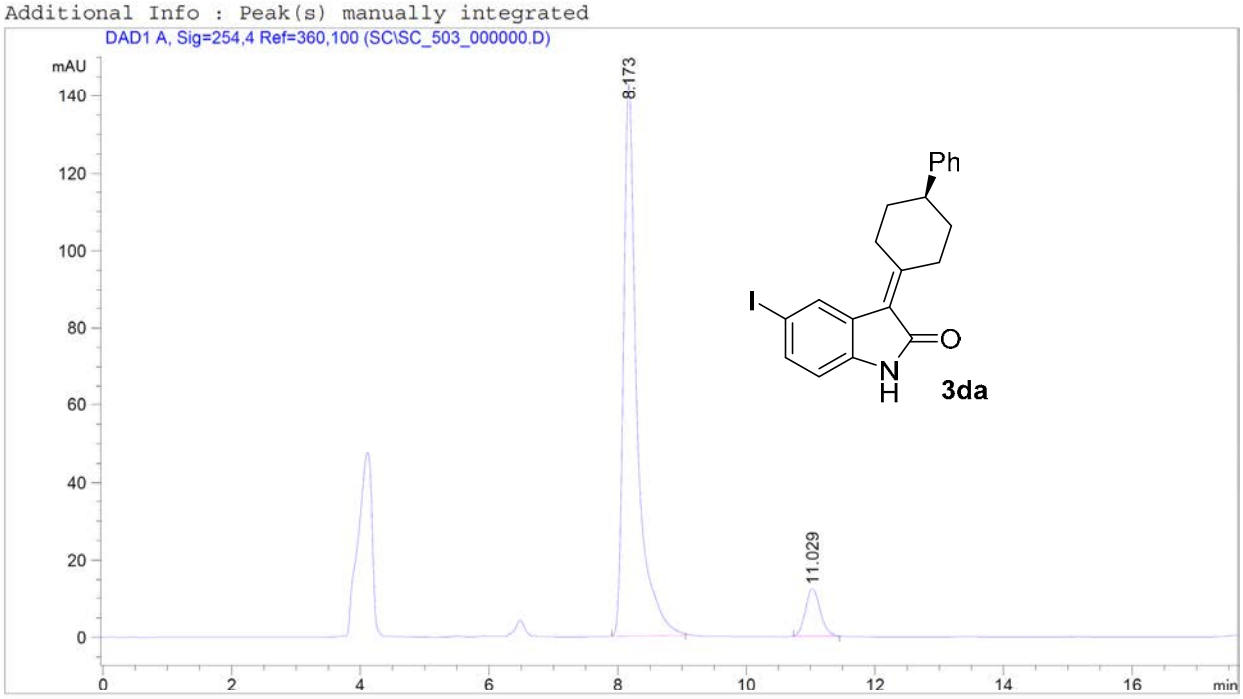



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.257 BB    0.1772  221.81863   19.42269  54.3842
   2  11.146 BB    0.2423  186.05493   11.90684  45.6158

Totals :                   407.87357   31.32953


==================================================================
                         *** End of Report ***

chiral 20/07/2018 13:37:28 Nico                          Page   1 of 1
```

Data File C:\CHEM32\2\DATA\SC\SC_503_000000.D
Sample Name: SC_503

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 1
Injection Date   : 04/12/2018 15:12:04
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/12/2018 15:10:16 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_503; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C
```

Additional Info : Peak(s) manually integrated



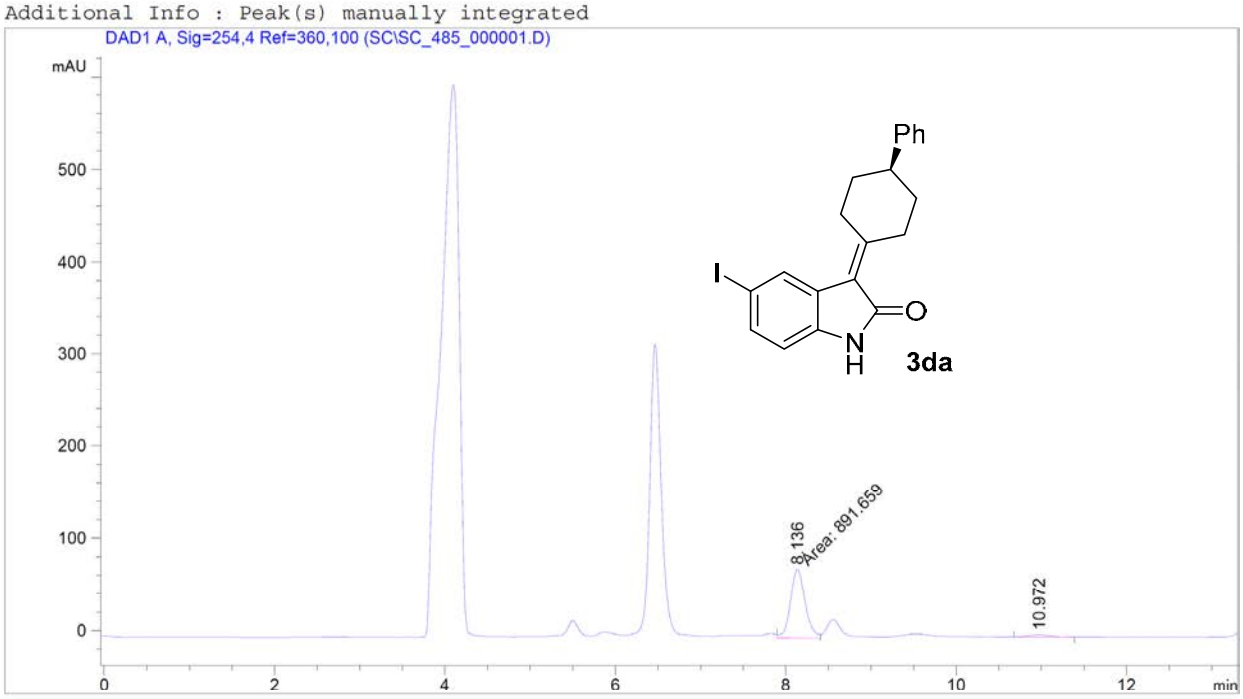

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.173 BB    0.2141 2079.92505  142.62016  91.2880
   2  11.029 BB    0.2476  198.49586   12.34740   8.7120

Totals :                  2278.42091  154.96756


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 11:55:57 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_485_000001.D
Sample Name: SC_485

```
==================================================================
Acq. Operator    : SIMONE
Acq. Instrument  : chiral                          Location : Vial 5
Injection Date   : 15/11/2018 15:41:56
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 15/11/2018 15:34:27 by SIMONE
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_485; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated



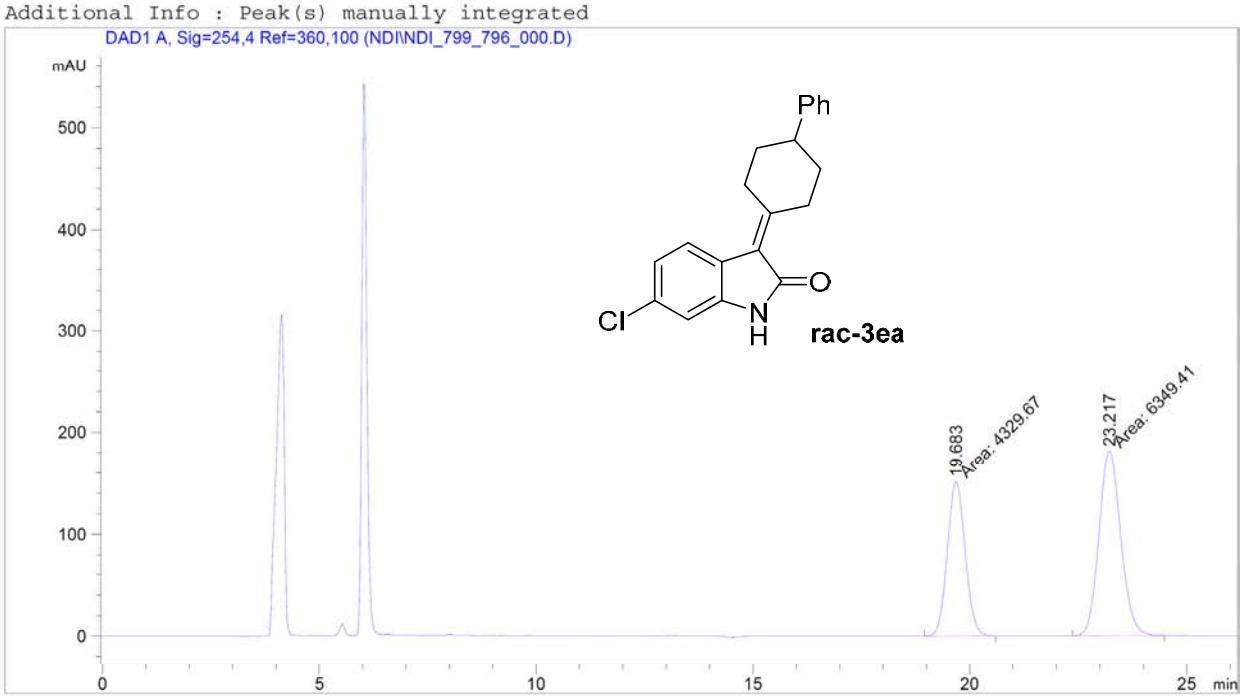

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.136 MM    0.1991  891.65875   74.64573  95.9631
   2  10.972 BB    0.2408   37.50932    2.44797   4.0369

Totals :                   929.16808   77.09370


==================================================================
                         *** End of Report ***
```

chiral 12/12/2018 11:41:58 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_799_796_000.D
Sample Name: NDI_799_796

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 95
Injection Date   : 01/06/2018 15:32:02
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 01/06/2018 15:29:59 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 04/06/2018 10:46:06 by Simone
                   (modified after loading)
Sample Info      : NDI_799_796; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



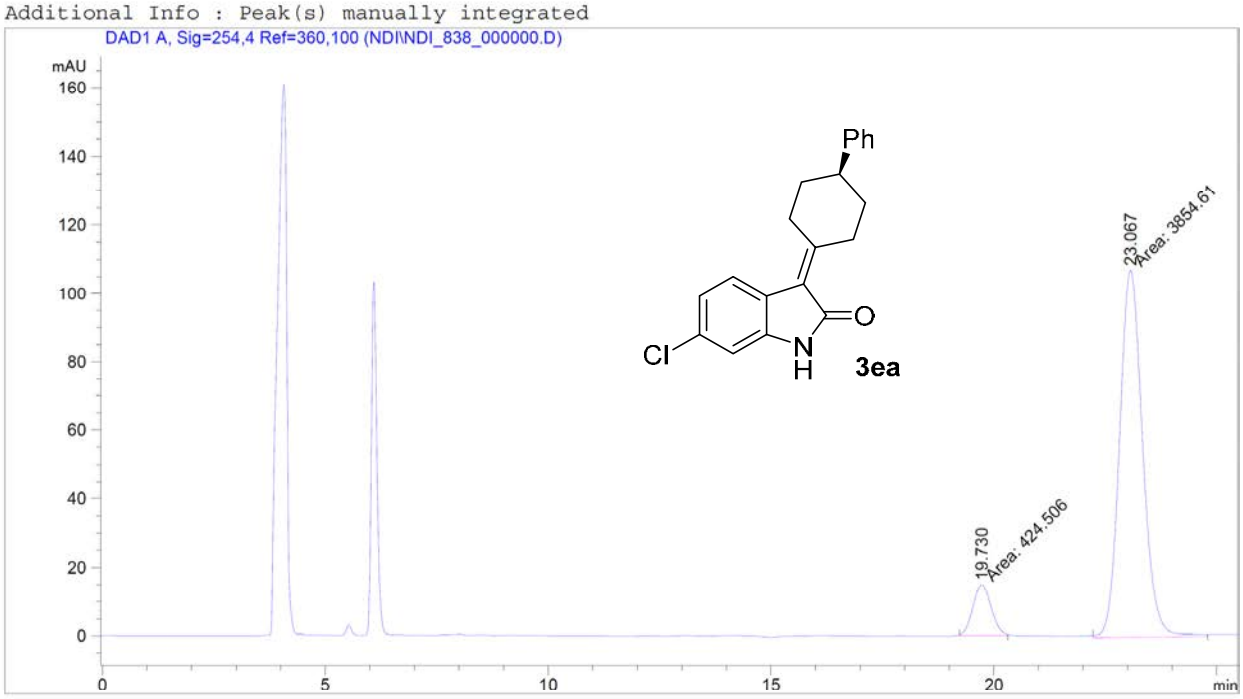

```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.683 MM    0.4769 4329.67432  151.31212  40.5435
   2  23.217 MM    0.5829 6349.40967  181.56064  59.4565

Totals :                  1.06791e4   332.87276


==================================================================
```

chiral 04/06/2018 10:55:26 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_838_000000.D
Sample Name: NDI_838

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 38
Injection Date   : 20/11/2018 15:10:24
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 20/11/2018 15:08:50 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : NDI_838; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated



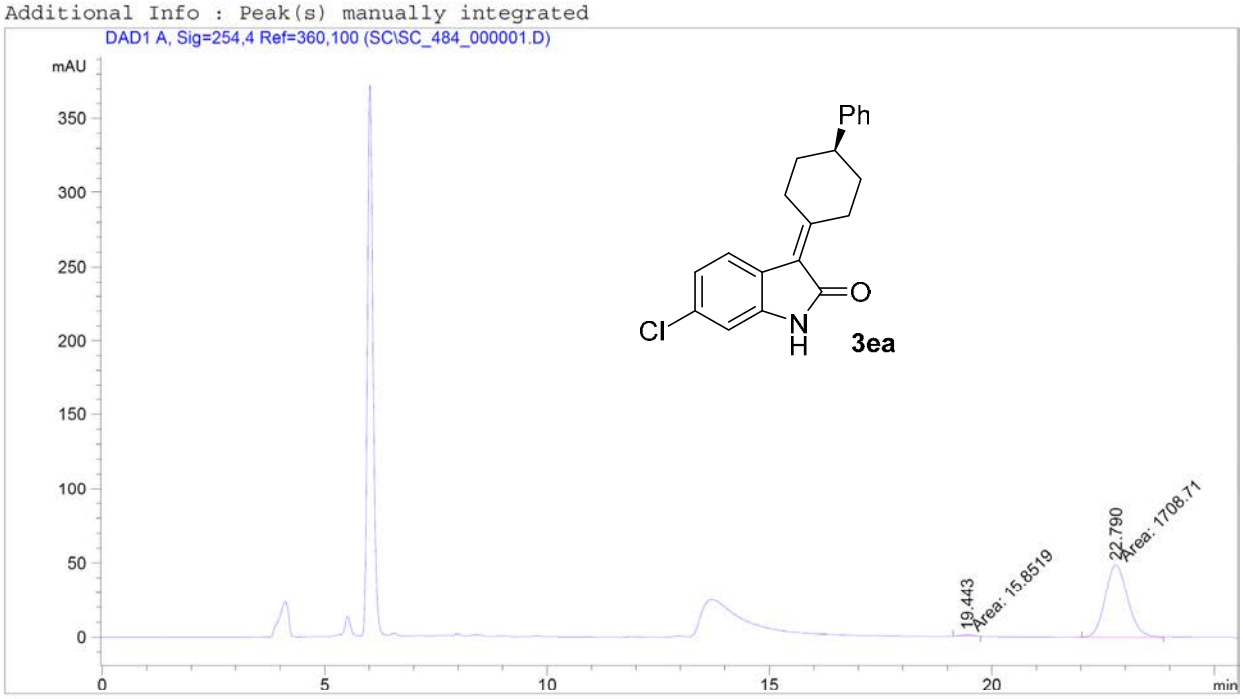

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  19.730 MM    0.4756  424.50613   14.87588   9.9204
   2  23.067 MM    0.5987 3854.60962  107.29633  90.0796

Totals :                  4279.11575  122.17220


==================================================================
                        *** End of Report ***
```

chiral 20/12/2018 11:52:18 Davide Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_484_000001.D
Sample Name: SC_484

```
==================================================================
Acq. Operator    : SIMONE
Acq. Instrument  : chiral                          Location : Vial 3
Injection Date   : 14/11/2018 12:08:34
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 14/11/2018 11:29:47 by SIMONE
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_484; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated



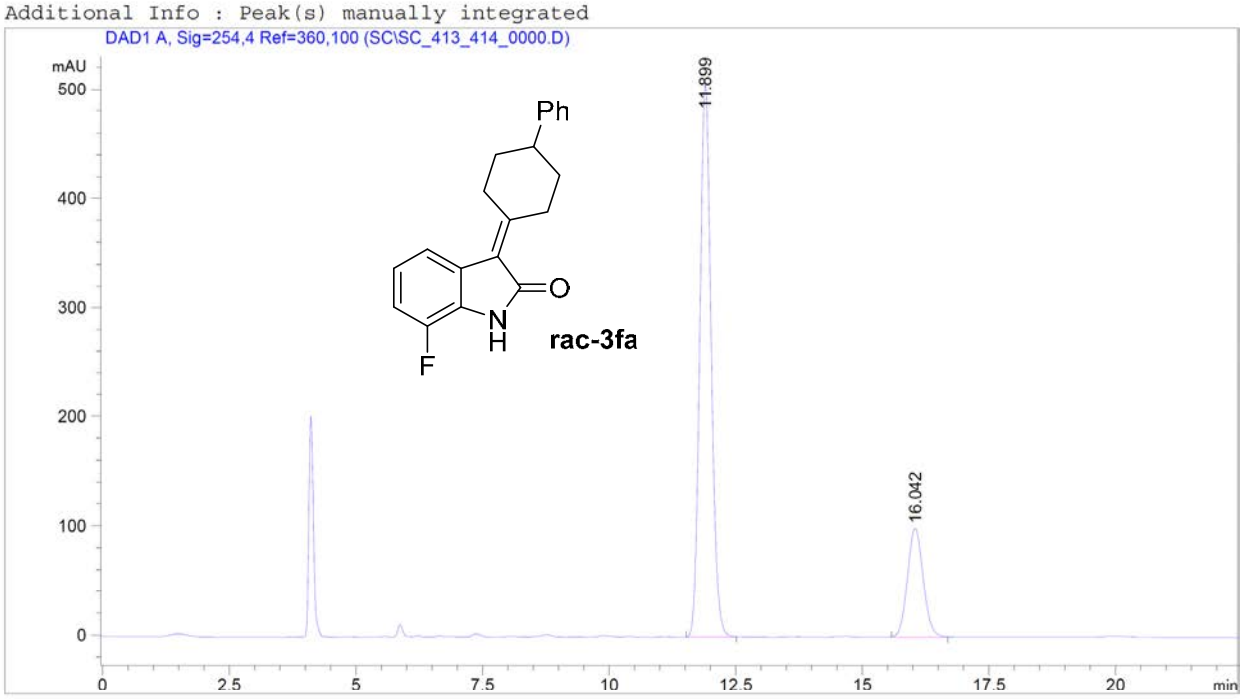

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height      Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  19.443 MM    0.3511   15.85189 7.52439e-1   0.9192
   2  22.790 MM    0.5839 1708.71289   48.77583  99.0808

Totals :                  1724.56479   49.52827


==================================================================
                          *** End of Report ***
```

chiral 12/12/2018 11:32:30 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_413_414_0000.D
Sample Name: SC_413_414

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 16
Injection Date   : 01/06/2018 17:45:40
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 01/06/2018 17:42:53 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : SC_413_414; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated

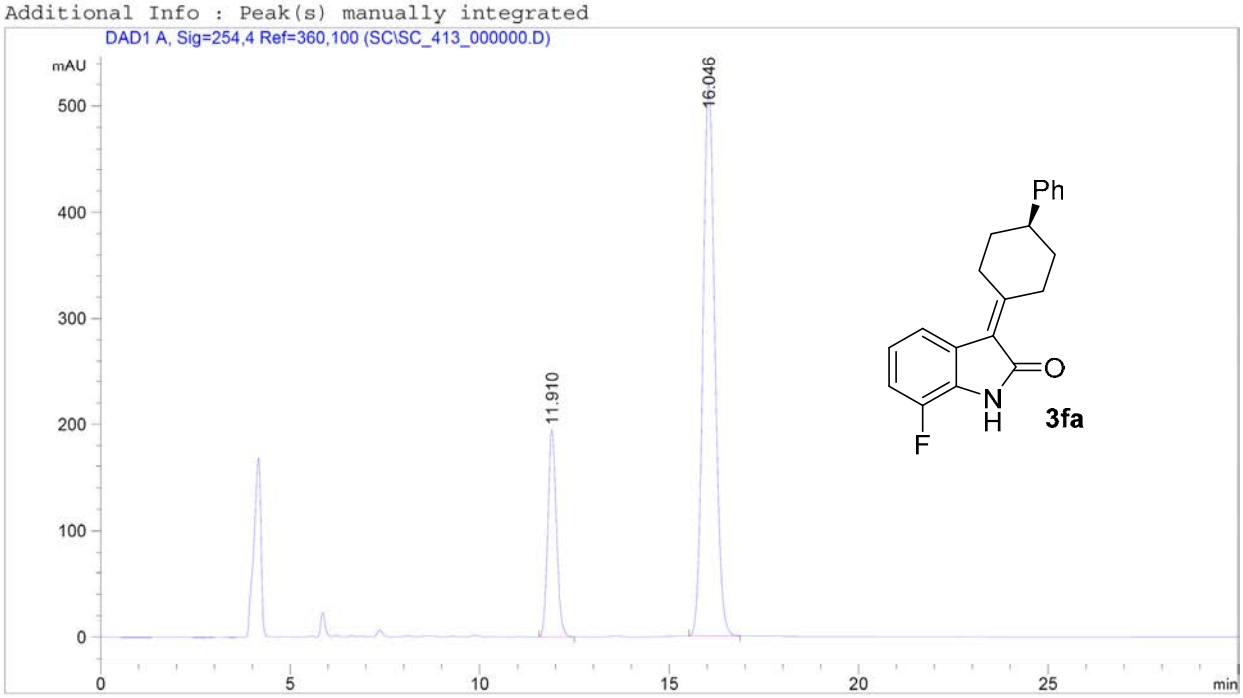



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  11.899 BB    0.2399 7888.19727  506.03595  78.5441
   2  16.042 BB    0.3343 2154.82056   99.66054  21.4559

Totals :                  1.00430e4   605.69649


==================================================================
                        *** End of Report ***
```

chiral 13/07/2018 14:51:31 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_413_000000.D
Sample Name: SC_413

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 14
Injection Date   : 01/06/2018 18:10:15
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 01/06/2018 18:08:28 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 13/07/2018 14:53:54 by Nico
                   (modified after loading)
Sample Info      : SC_413; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi

Additional Info : Peak(s) manually integrated
```

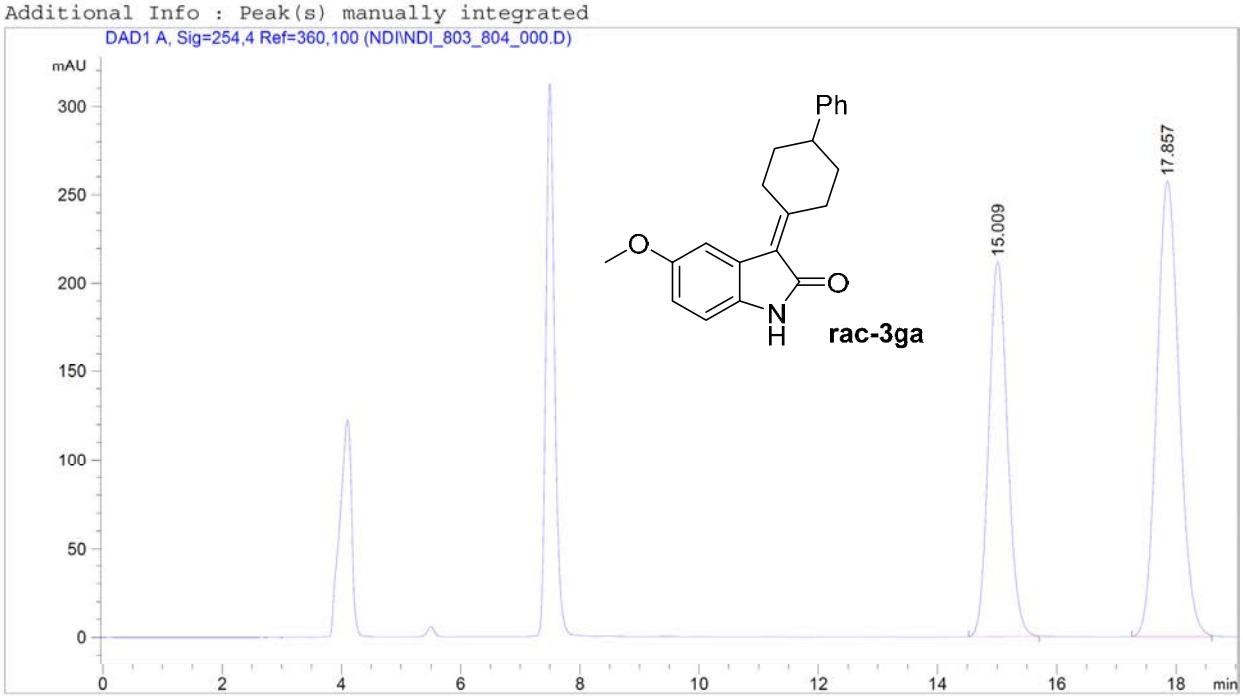



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  11.910 BB    0.2438 3066.86475  194.62915  21.1992
   2  16.046 BB    0.3400 1.14000e4   519.55835  78.8008

Totals :                  1.44669e4   714.18750


==================================================================
```

chiral 13/07/2018 14:54:21 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_803_804_000.D
Sample Name: NDI_803_804

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 2
Injection Date   : 12/06/2018 13:58:51
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 12/06/2018 13:37:14 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 12/06/2018 14:46:50 by Nico
                   (modified after loading)
Sample Info      : NDI_803_804; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi

Additional Info : Peak(s) manually integrated
```

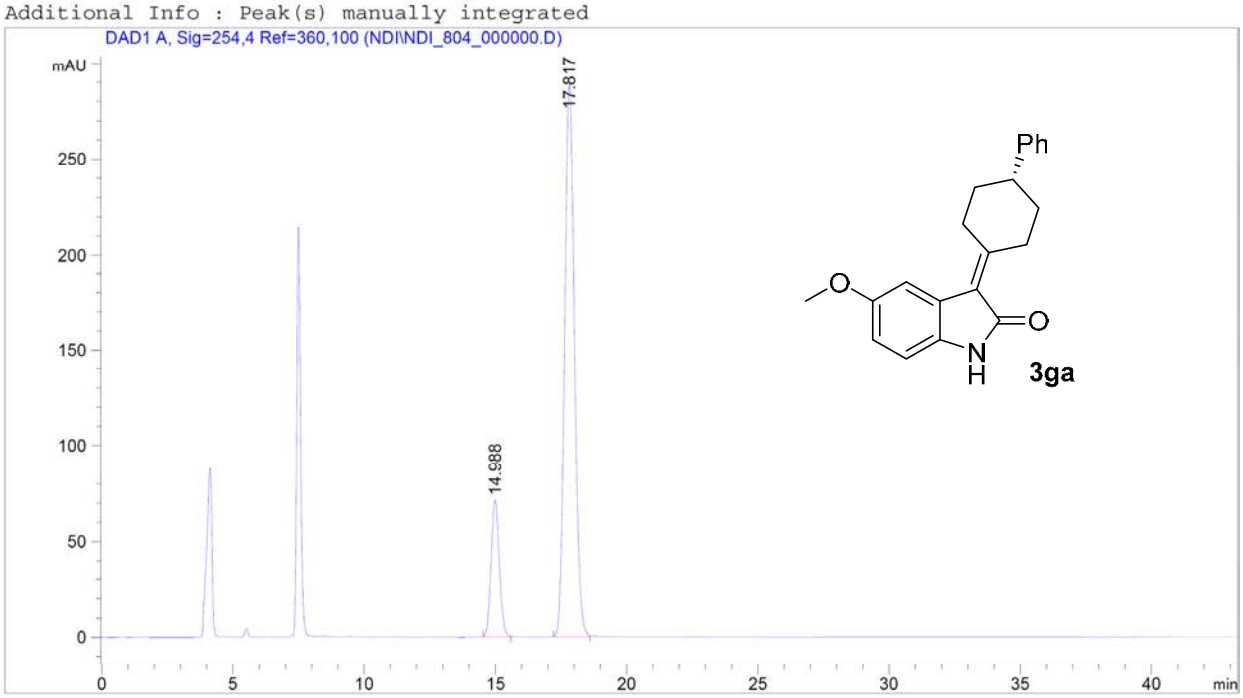



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  15.009 BB    0.3379 4622.25439  212.41277  40.7445
   2  17.857 BBA   0.4045 6722.24072  257.55582  59.2555

Totals :                  1.13445e4   469.96858


==================================================================
```

chiral 12/06/2018 14:47:22 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_804_000000.D
Sample Name: NDI_804

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 4
Injection Date   : 12/06/2018 14:42:47
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 12/06/2018 14:41:20 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 12/06/2018 14:46:50 by Nico
                   (modified after loading)
Sample Info      : NDI_804; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi


Additional Info : Peak(s) manually integrated
```

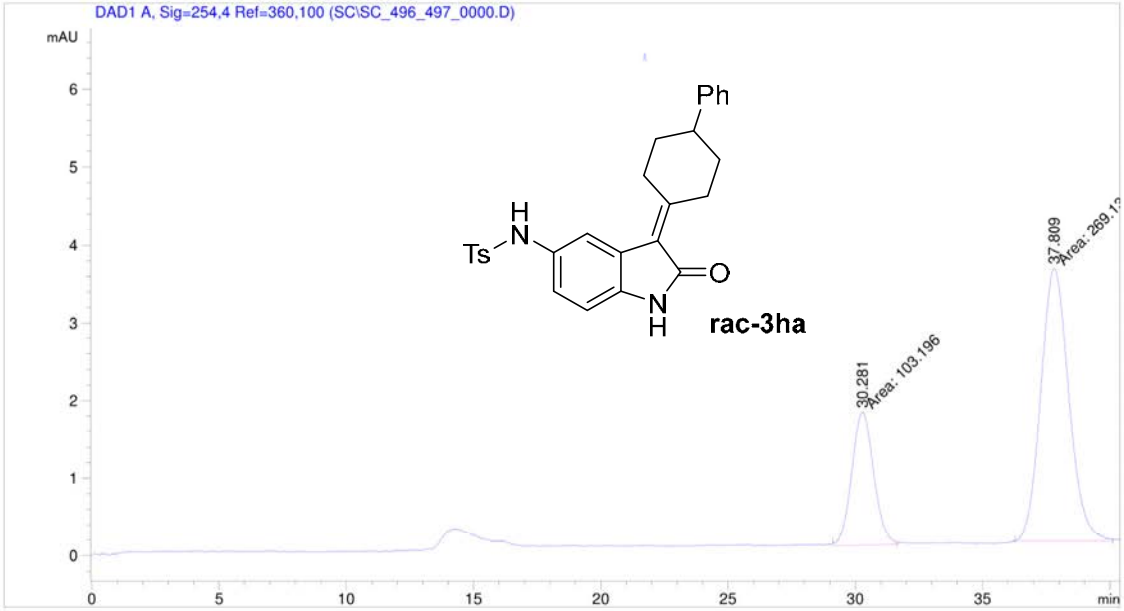



```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  14.988 BB    0.3334 1536.46484   71.29188  17.0042
   2  17.817 BBA   0.4027 7499.31885  289.01938  82.9958

Totals :                  9035.78369  360.31126


==================================================================
```

chiral 12/06/2018 15:27:01 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_496_497_0000.D
Sample Name: SC_496_497

```
==========================================================================
Acq. Operator   : Simone
Acq. Instrument : chiral                          Location : Vial 1
Injection Date  : 20/12/2018 12:43:46
                                                Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed    : 20/12/2018 12:42:19 by Simone
                  (modified after loading)
Analysis Method : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed    : 29/11/2018 09:46:42 by Simone
Sample Info     : SC_496_497; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C


Additional Info : Peak(s) manually integrated
```



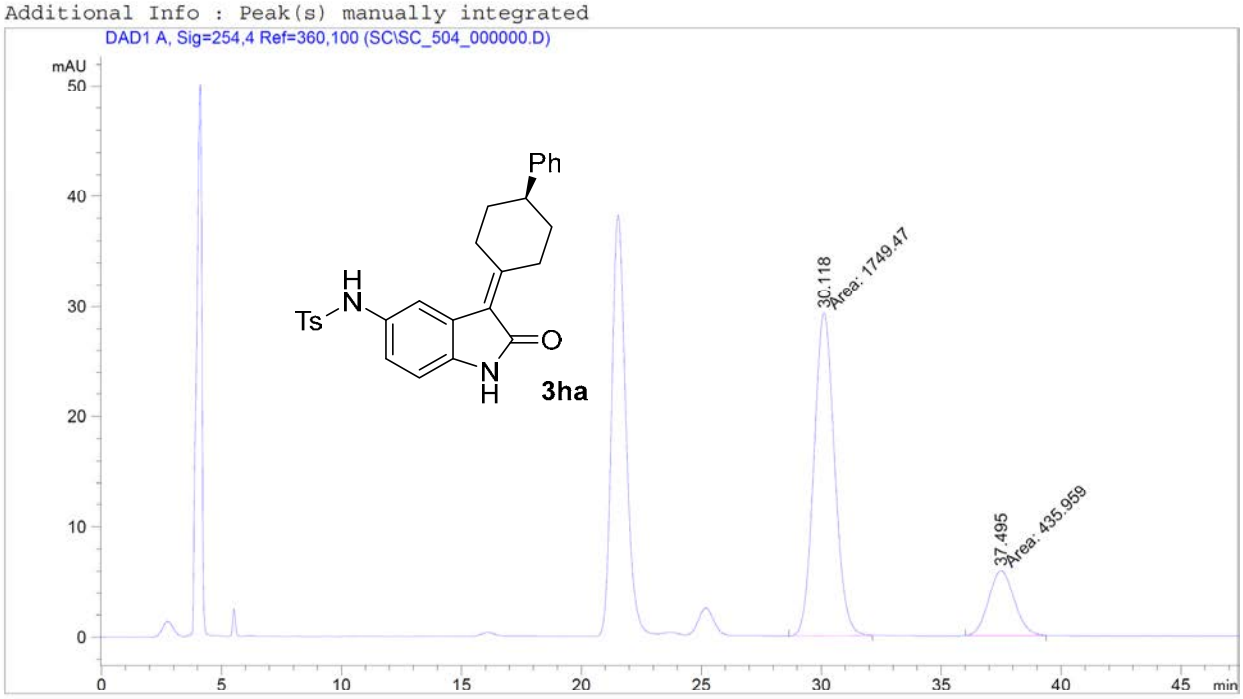

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  30.281 MM    1.0014  103.19575    1.71750  27.7158
   2  37.809 MM    1.2768  269.13910    3.51327  72.2842

Totals :                   372.33485    5.23077


==========================================================================
                           *** End of Report ***
```

chiral 20/12/2018 15:47:38 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_504_000000.D
Sample Name: SC_504

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 2
Injection Date   : 04/12/2018 15:31:56
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/12/2018 15:30:07 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_504; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C
```

Additional Info : Peak(s) manually integrated

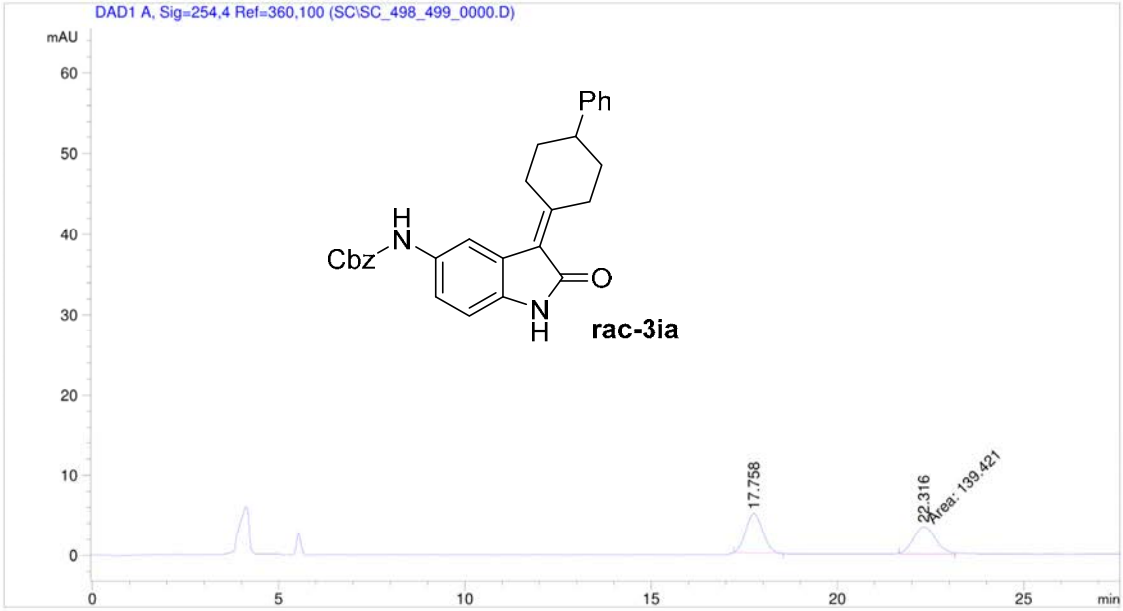



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  30.118 MM    0.9956 1749.47131   29.28721  80.0516
   2  37.495 MM    1.2314  435.95865    5.90067  19.9484

Totals :                  2185.42996   35.18788


==================================================================
                        *** End of Report ***
```

chiral 20/12/2018 12:04:45 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_498_499_0000.D
Sample Name: SC_498_499

```
==========================================================================
Acq. Operator   : Simone
Acq. Instrument : chiral                          Location : Vial 2
Injection Date  : 20/12/2018 15:39:42
                                                Inj Volume : 10.0 µl
Acq. Method     : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed    : 20/12/2018 15:35:37 by Simone
                  (modified after loading)
Analysis Method : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed    : 29/11/2018 09:46:42 by Simone
Sample Info     : SC_498_499; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C


Additional Info : Peak(s) manually integrated
```



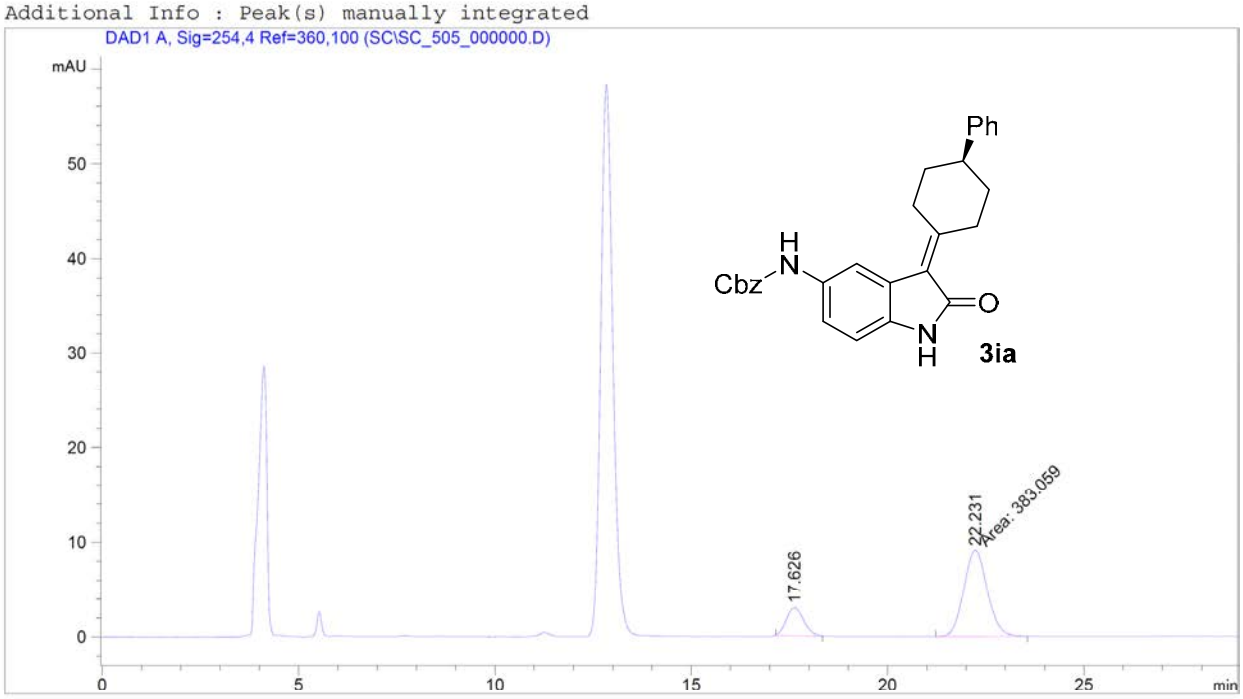

```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  17.758 BB    0.4848  157.45102    4.95364  53.0367
   2  22.316 MM    0.6811  139.42084    3.41176  46.9633

Totals :                   296.87186    8.36540


==========================================================================
                           *** End of Report ***
```

chiral 20/12/2018 16:08:57 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_505_000000.D
Sample Name: SC_505

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 3
Injection Date   : 04/12/2018 16:21:11
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/12/2018 16:19:40 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_505; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C
```

Additional Info : Peak(s) manually integrated

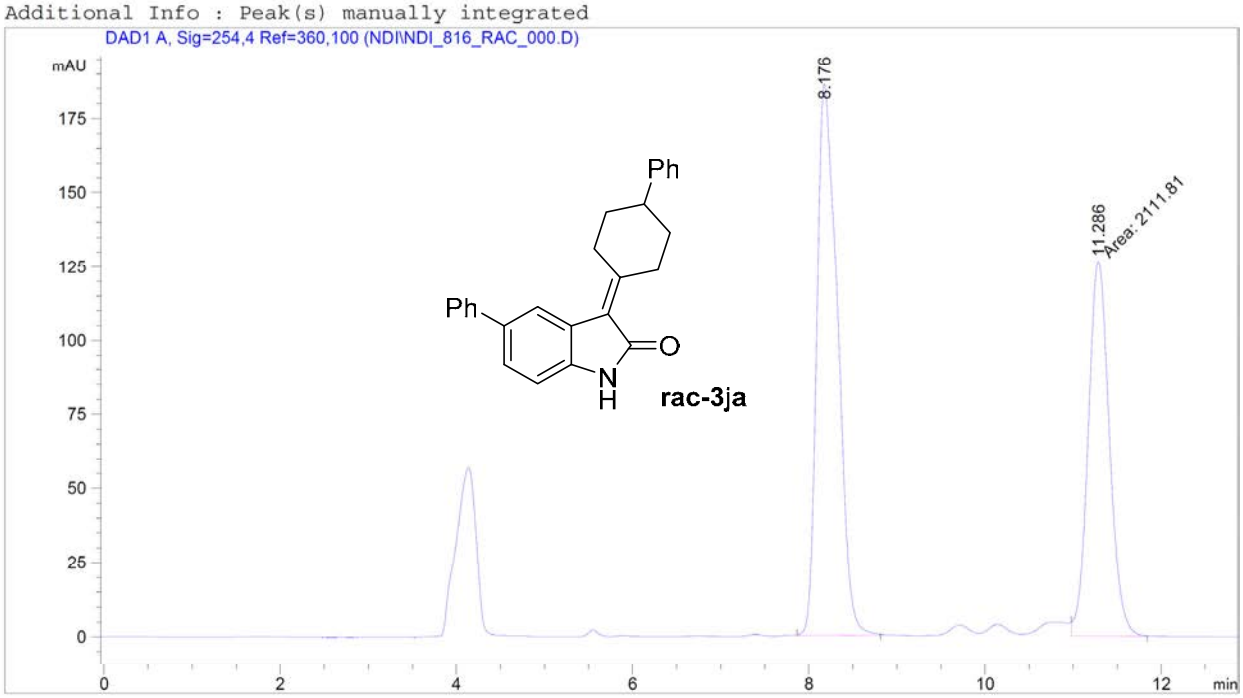



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  17.626 BB    0.4636   91.06041    2.93769  19.2062
   2  22.231 MM    0.6999  383.05905    9.12227  80.7938

Totals :                   474.11946   12.05996


==================================================================
                         *** End of Report ***
```

chiral 20/12/2018 12:06:31 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_816_RAC_000.D
Sample Name: NDI_816_rac

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 15
Injection Date   : 19/07/2018 17:37:33
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 19/07/2018 17:36:15 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : NDI_816_rac; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```



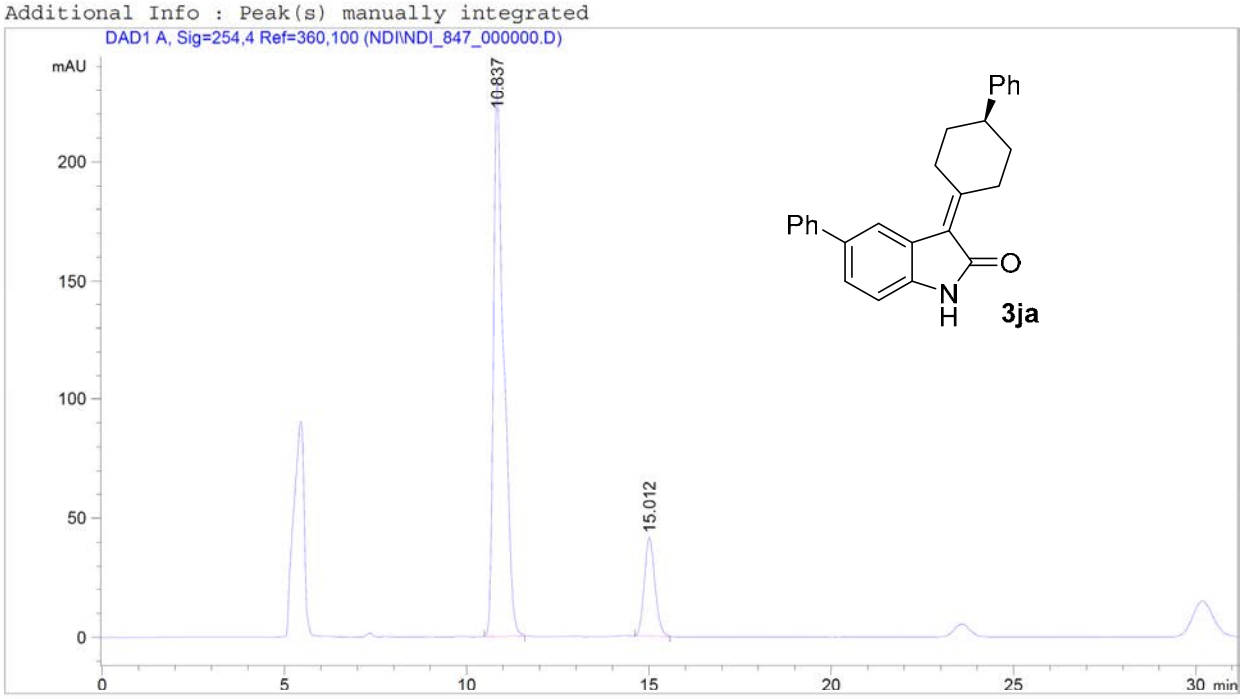

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.176 BB    0.2317 3026.90210  186.11856  58.9039
   2  11.286 FM    0.2778 2111.80640  126.67872  41.0961

Totals :                  5138.70850  312.79728


==================================================================
```

chiral 20/07/2018 11:43:53 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_847_000000.D
Sample Name: NDI_847

```
==================================================================
Acq. Operator    : NIco
Acq. Instrument  : chiral                          Location : Vial 47
Injection Date   : 07/12/2018 17:20:57
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 07/12/2018 17:06:45 by NIco
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : NDI_847; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25°C
```

Additional Info : Peak(s) manually integrated

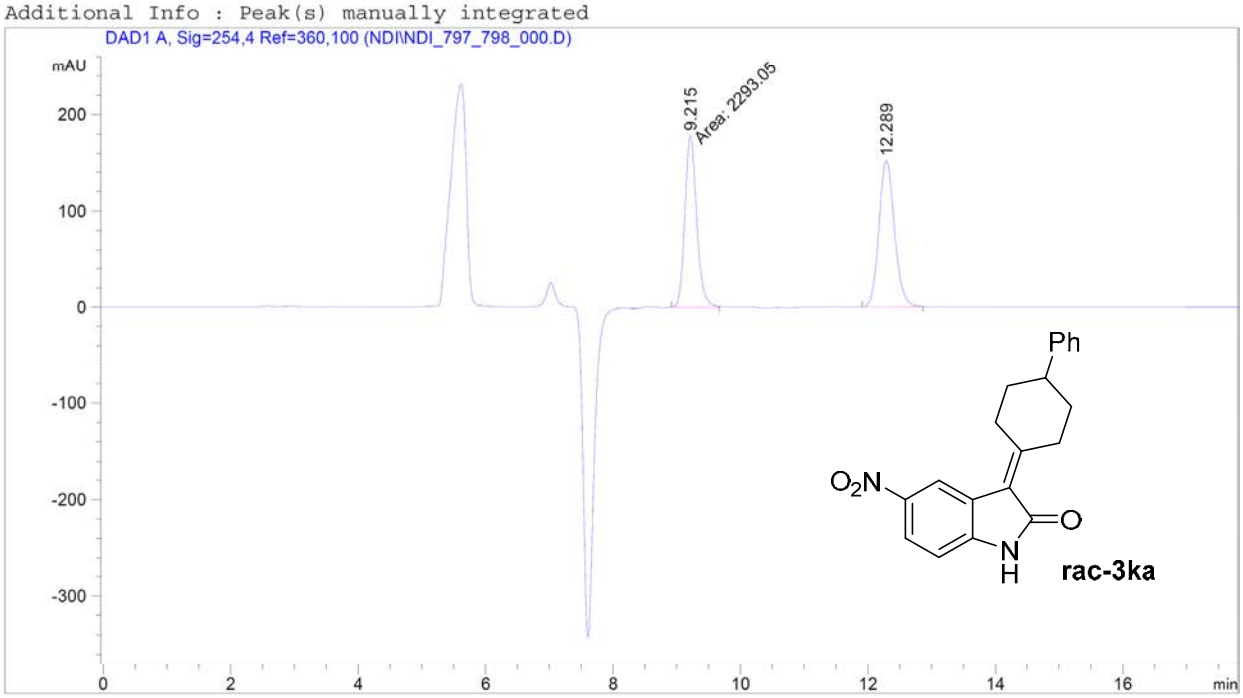



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  10.837 BB    0.2760 4495.42041  232.09929  84.1744
   2  15.012 BB    0.3143  845.18542   41.37948  15.8256

Totals :                  5340.60583  273.47877


==================================================================
                        *** End of Report ***
```

chiral 20/12/2018 12:21:17 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_797_798_000.D
Sample Name: NDI_797_798

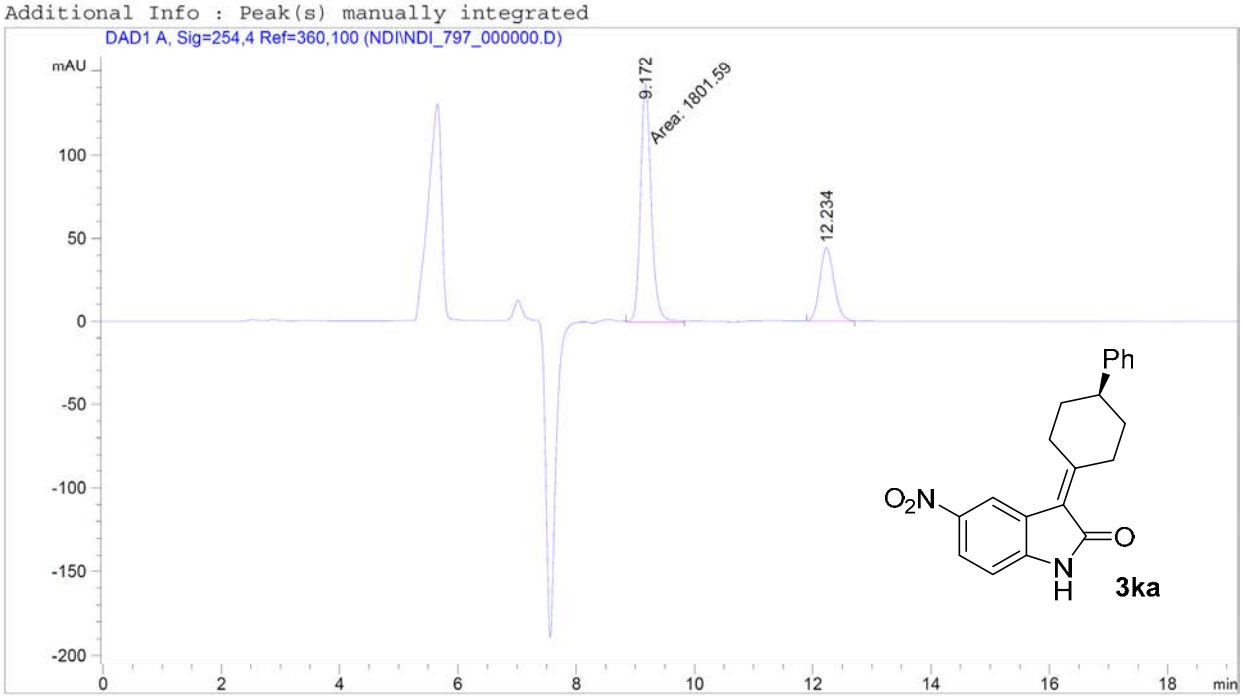
```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 100
Injection Date   : 04/06/2018 10:06:52
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 04/06/2018 10:03:41 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 04/06/2018 10:46:06 by Simone
                   (modified after loading)
Sample Info      : NDI_797_798; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi


Additional Info : Peak(s) manually integrated
```




```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.215 MM    0.2138 2293.04565  178.73656  47.0996
   2  12.289 BB    0.2615 2575.46143  152.10397  52.9004

Totals :                  4868.50708  330.84053


==================================================================

chiral 04/06/2018 10:56:12 Simone                          Page   1 of 1
```

Data File C:\CHEM32\2\DATA\NDI\NDI_797_000000.D
Sample Name: NDI_797

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 97
Injection Date   : 04/06/2018 10:27:28
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 04/06/2018 10:25:04 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 04/06/2018 10:46:06 by Simone
                   (modified after loading)
Sample Info      : NDI_797; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi


Additional Info : Peak(s) manually integrated
```



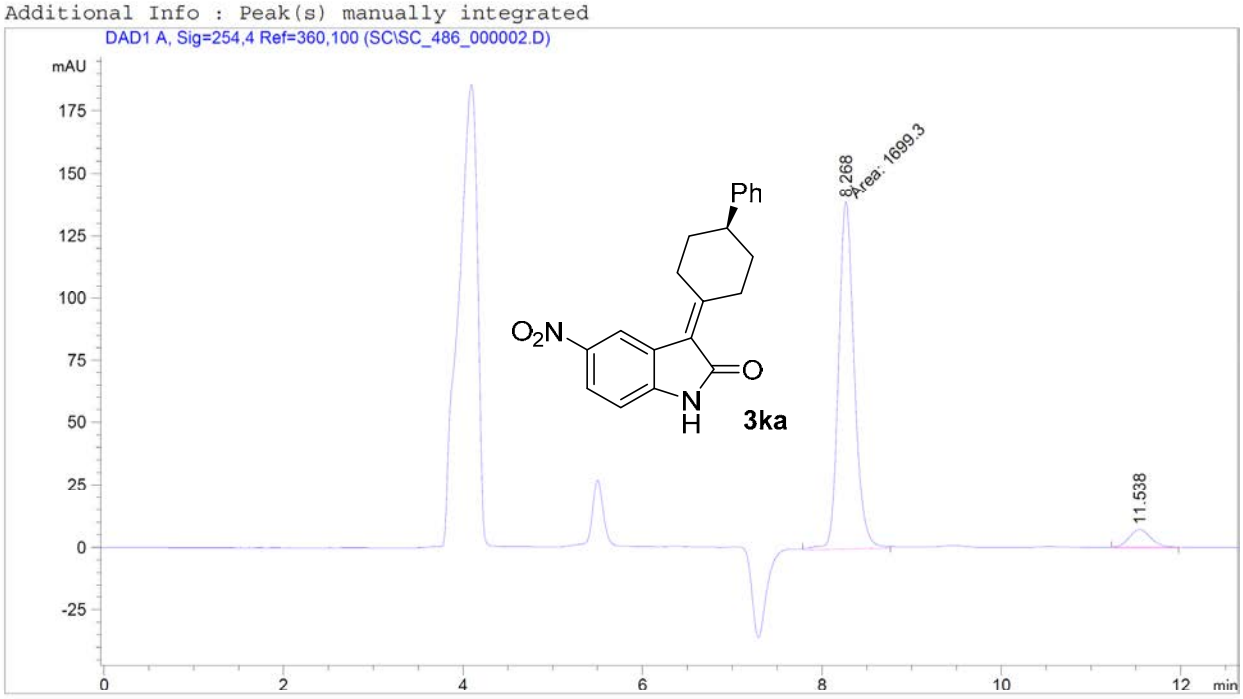

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   9.172 MM    0.2104 1801.59180  142.69514  70.9232
   2  12.234 BB    0.2577  738.60980   44.48778  29.0768

Totals :                  2540.20160  187.18293


==================================================================
```

chiral 04/06/2018 11:10:58 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_486_000002.D
Sample Name: SC_486

```
==================================================================
Acq. Operator    : SIMONE
Acq. Instrument  : chiral                          Location : Vial 6
Injection Date   : 16/11/2018 10:21:12
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 16/11/2018 10:15:40 by SIMONE
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_486; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated

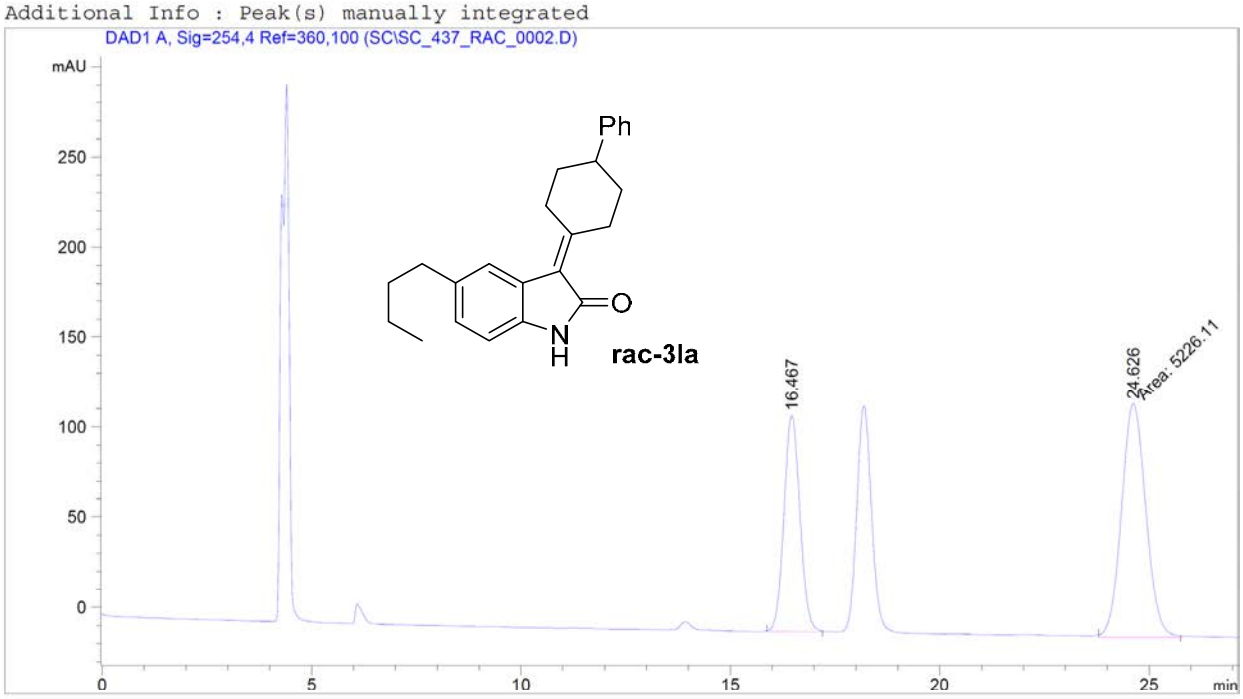



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.268 MM    0.2035 1699.29688  139.17642  93.4252
   2  11.538 BB    0.2601  119.58881    7.11445   6.5748

Totals :                  1818.88569  146.29087


==================================================================
                        *** End of Report ***
```

Data File C:\CHEM32\2\DATA\SC\SC_437_RAC_0002.D
Sample Name: SC_437_rac

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 37
Injection Date   : 19/07/2018 13:58:00
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 19/07/2018 13:52:39 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : SC_437_rac; IC; Hex/IPA 80/20; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated



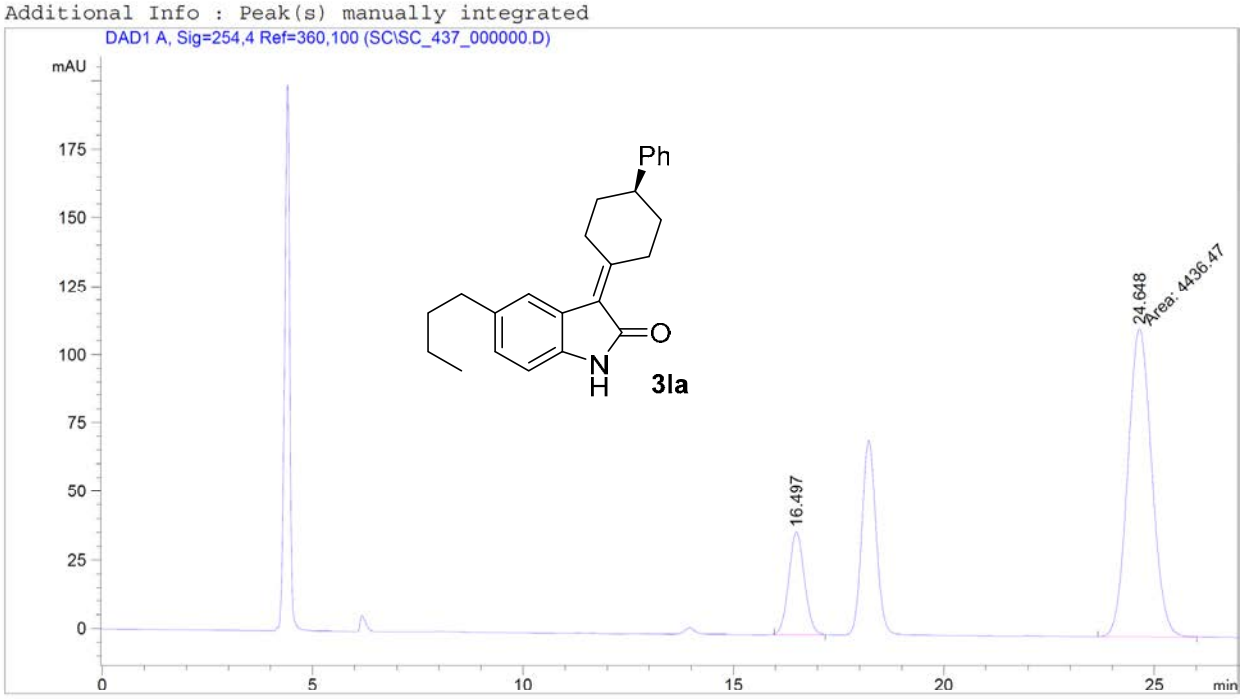

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  16.467 BB    0.4106 3165.79004  119.68980  37.7244
   2  24.626 MM    0.6736 5226.10742  129.30026  62.2756

Totals :                  8391.89746  248.99006


==================================================================
                         *** End of Report ***
```

chiral 19/07/2018 14:55:50 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_437_000000.D
Sample Name: SC_437

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 38
Injection Date   : 19/07/2018 14:30:26
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 19/07/2018 14:25:31 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_437; IC; Hex/IPA 90/10; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated

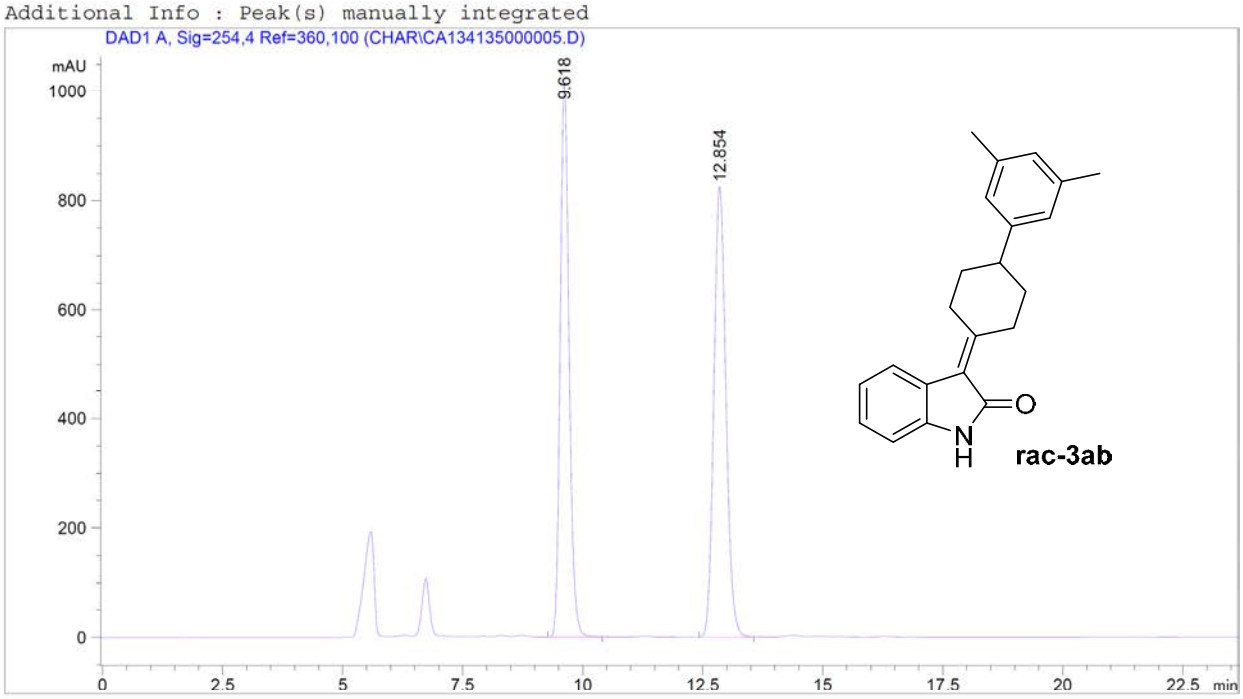



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  16.497 BB    0.4009  972.55554   37.45436  17.9802
   2  24.648 MM    0.6581 4436.46729  112.35944  82.0198

Totals :                   5409.02283  149.81380


==================================================================
                        *** End of Report ***
```

chiral 20/12/2018 12:41:49 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA134135000005.D
Sample Name: CA_134_135

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 65
Injection Date   : 15/06/2018 13:59:32
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 15/06/2018 13:57:33 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : CA_134_135 ; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi


Additional Info : Peak(s) manually integrated
```



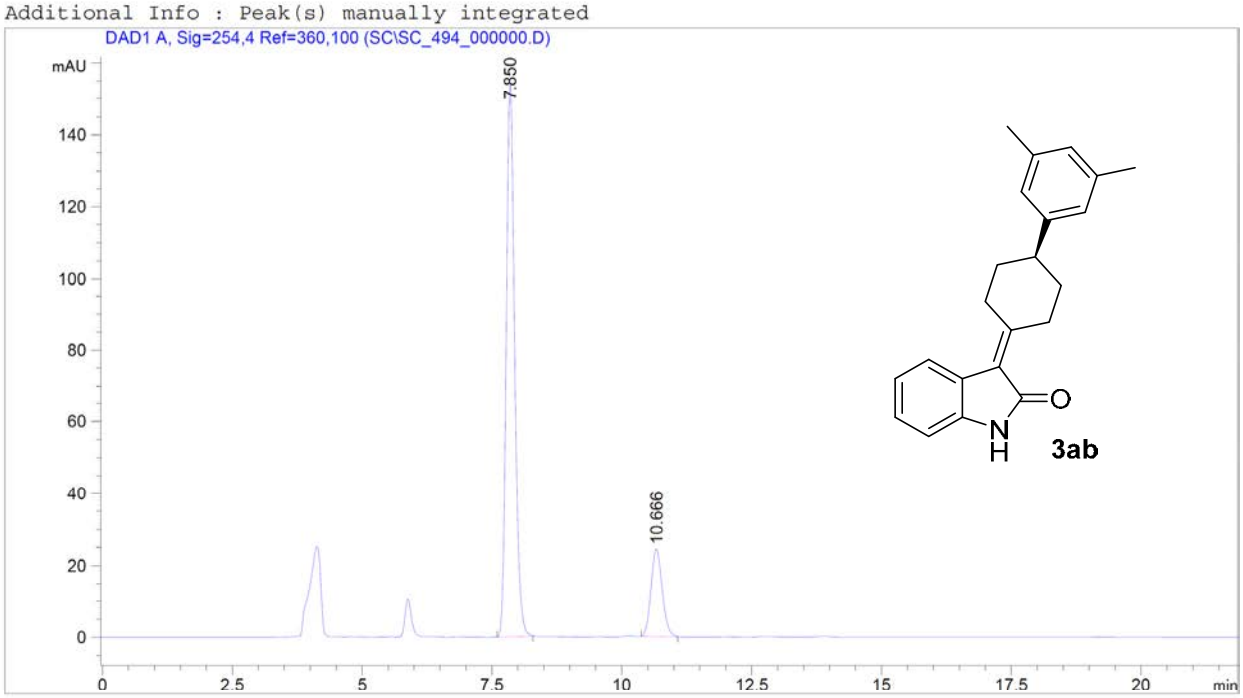

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   9.618 VB    0.1983 1.30392e4  1011.99530  47.5259
   2  12.854 BB    0.2694 1.43968e4   825.90253  52.4741

Totals :                  2.74359e4  1837.89783


==================================================================
                        *** End of Report ***
```

chiral 11/07/2018 10:06:05 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_494_000000.D
Sample Name: SC_494

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 67
Injection Date   : 21/11/2018 13:31:48
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 21/11/2018 13:28:59 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_494; AD-H 70:30 Hex/IPA; 0.8 ml/min; 25 °C
```

Additional Info : Peak(s) manually integrated



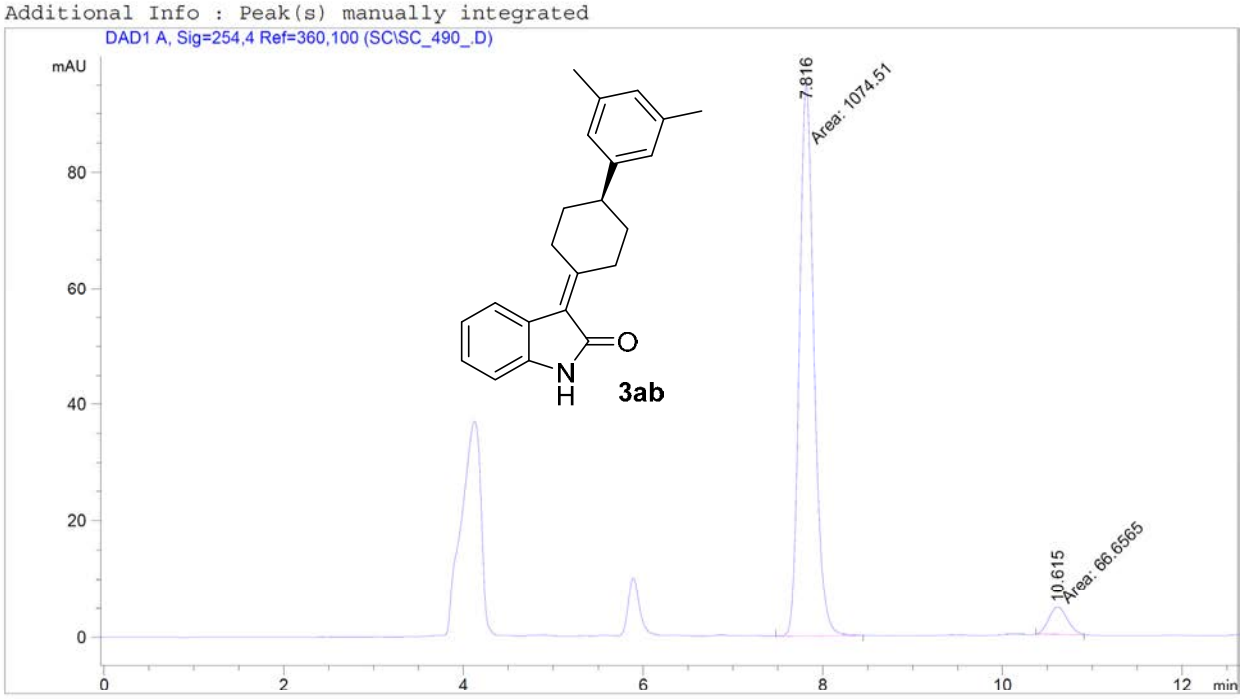

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   7.850 BB    0.1732 1731.16333  153.90436  82.5402
   2  10.666 BB    0.2312  366.19507   24.38451  17.4598

Totals :                  2097.35840  178.28886


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 12:27:16 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_490_.D
Sample Name: SC_490

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 63
Injection Date   : 21/11/2018 09:46:51
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 21/11/2018 09:29:59 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_490; AD-H 70:30 Hex/IPA; 0.8 ml/min; 25 °C
```

Additional Info : Peak(s) manually integrated

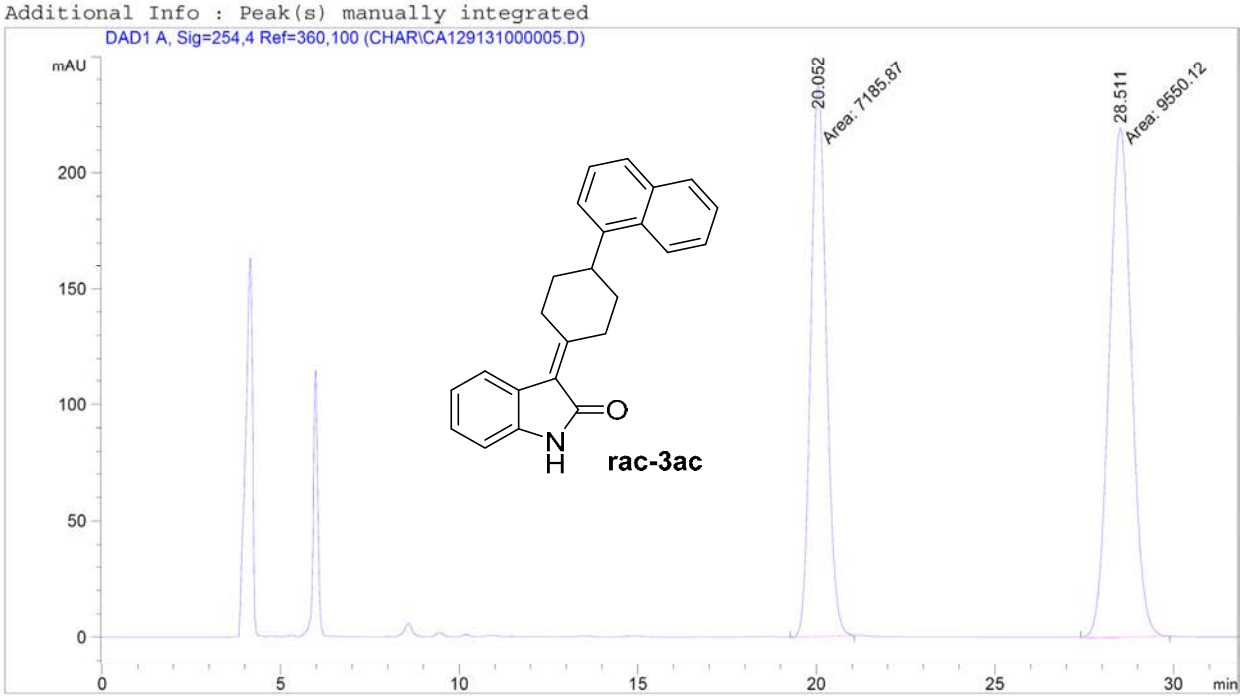



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   7.816 MM    0.1886 1074.51086   94.94832  94.1589
   2  10.615 MM    0.2382   66.65648    4.66392   5.8411

Totals :                  1141.16734   99.61224


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 12:25:51 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA129131000005.D
Sample Name: CA_129_131

```
==========================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 54
Injection Date   : 14/06/2018 10:12:12
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 14/06/2018 10:10:16 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 10/07/2018 11:34:07 by stefano
                   (modified after loading)
Sample Info      : CA_129_131 ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi


Additional Info : Peak(s) manually integrated
```

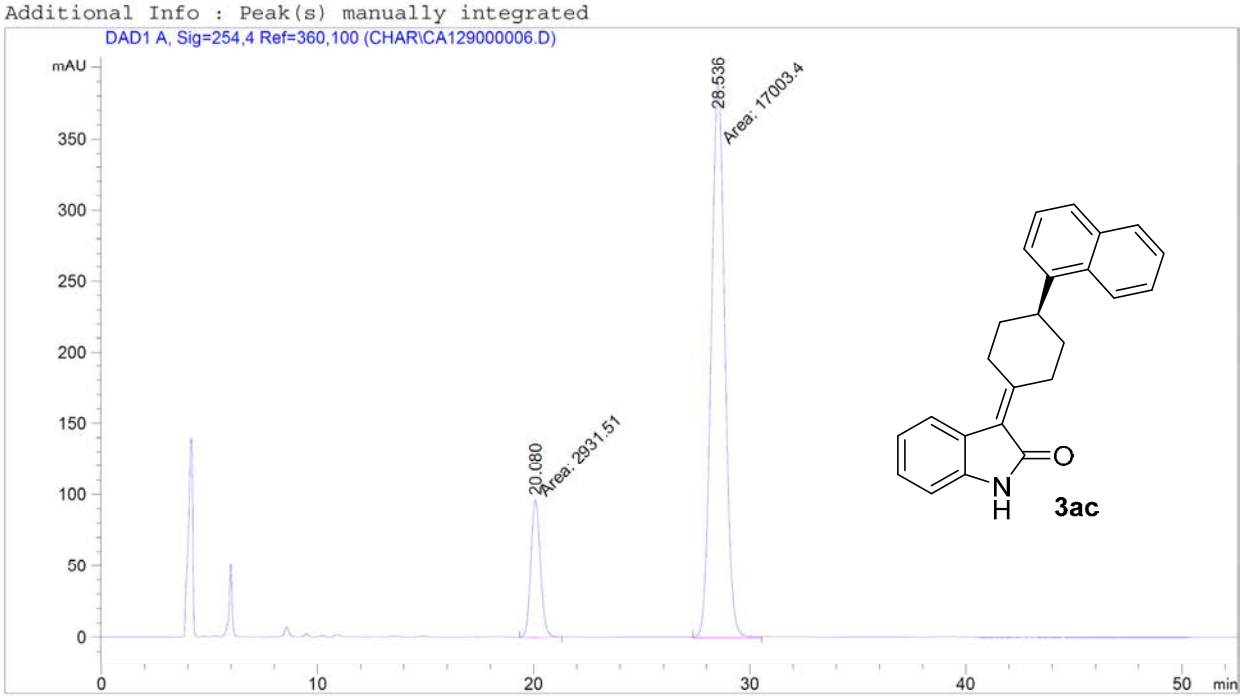



```
==========================================================================
                           Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  20.052 MM    0.5031 7185.87402  238.04343  42.9366
   2  28.511 MM    0.7254 9550.12305  219.41803  57.0634

Totals :                  1.67360e4   457.46146


==========================================================================

chiral 10/07/2018 11:43:35 stefano                          Page   1 of 1
```

Data File C:\CHEM32\2\DATA\CHAR\CA129000006.D
Sample Name: CA_129

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 55
Injection Date   : 14/06/2018 10:46:01
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 14/06/2018 10:44:23 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 10/07/2018 11:34:07 by stefano
                   (modified after loading)
Sample Info      : CA_129_ ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



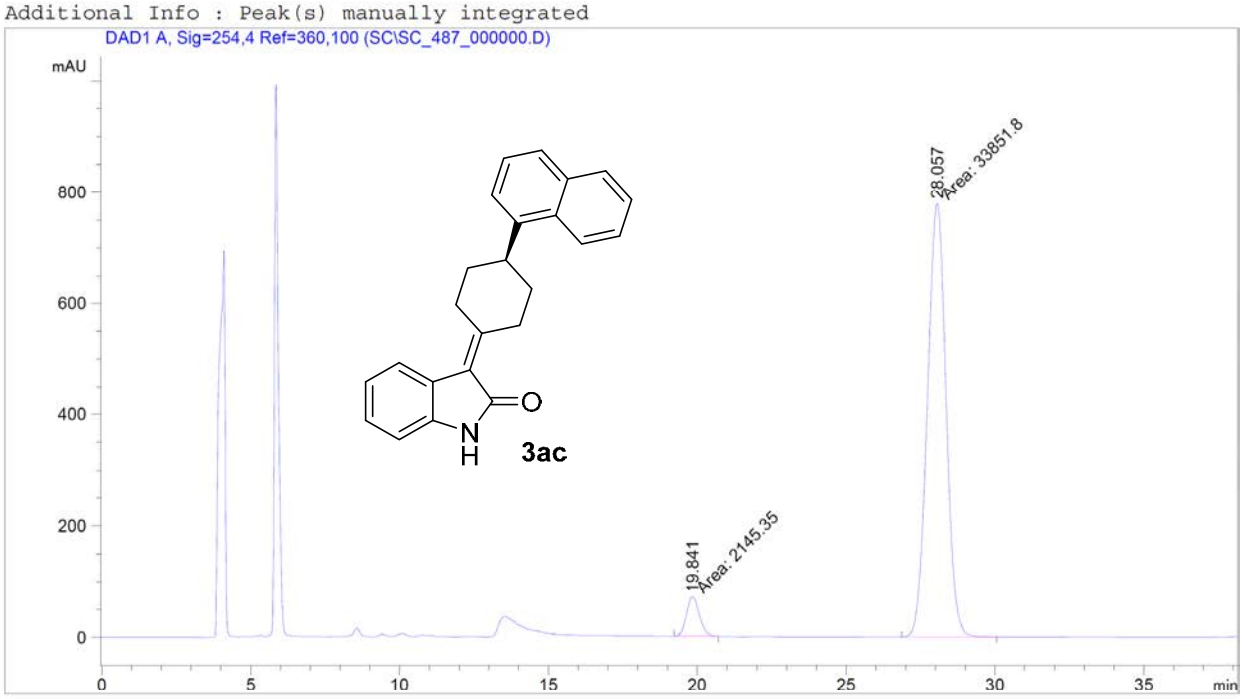

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  20.080 MM    0.5071 2931.50513   96.34200  14.7054
   2  28.536 MM    0.7287 1.70034e4   388.87463  85.2946

Totals :                  1.99349e4   485.21664


==================================================================
```

chiral 10/07/2018 11:44:30 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_487_000000.D
Sample Name: SC_487

```
==================================================================
Acq. Operator    : SIMONE
Acq. Instrument  : chiral                          Location : Vial 7
Injection Date   : 15/11/2018 16:53:04
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 15/11/2018 16:46:14 by SIMONE
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_487; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;
```

Additional Info : Peak(s) manually integrated

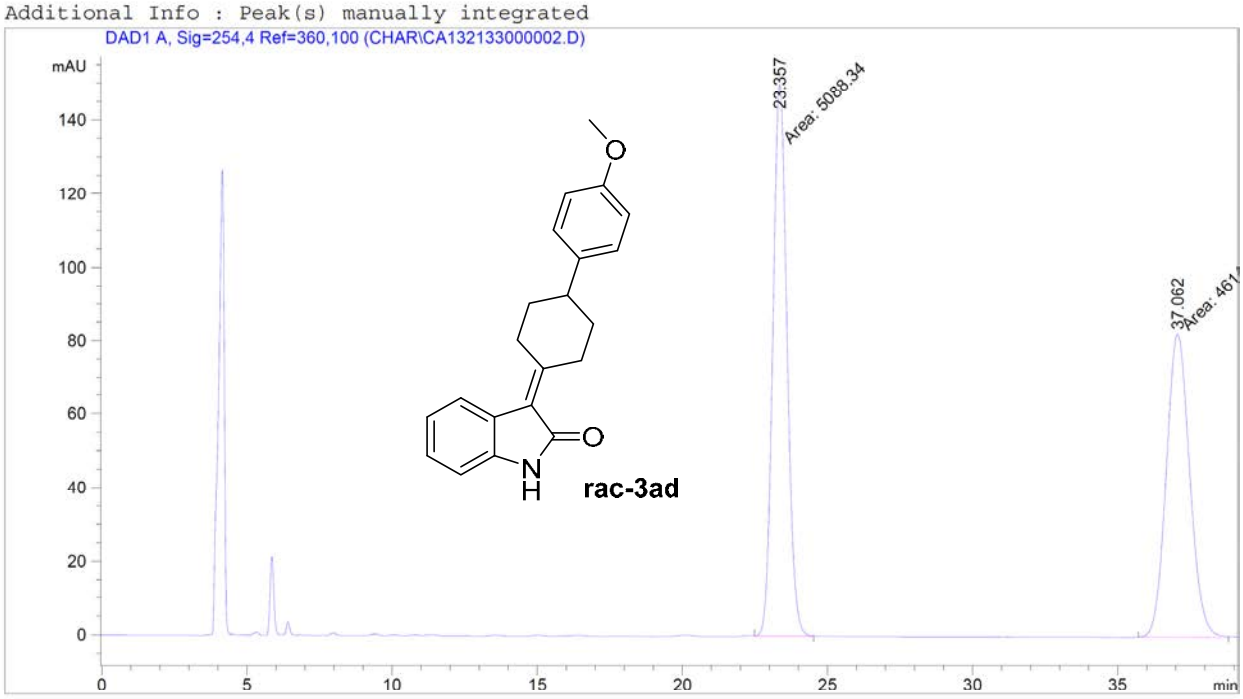



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  19.841 MM    0.5071 2145.35278   70.51295   5.9598
   2  28.057 MM    0.7238 3.38518e4   779.45020  94.0402

Totals :                  3.59972e4   849.96315


==================================================================
                         *** End of Report ***
```

Data File C:\CHEM32\2\DATA\CHAR\CA132133000002.D
Sample Name: CA_132_133

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 62
Injection Date   : 15/06/2018 11:47:24
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 15/06/2018 11:23:27 by Luca
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : CA_132_133 ; IC; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



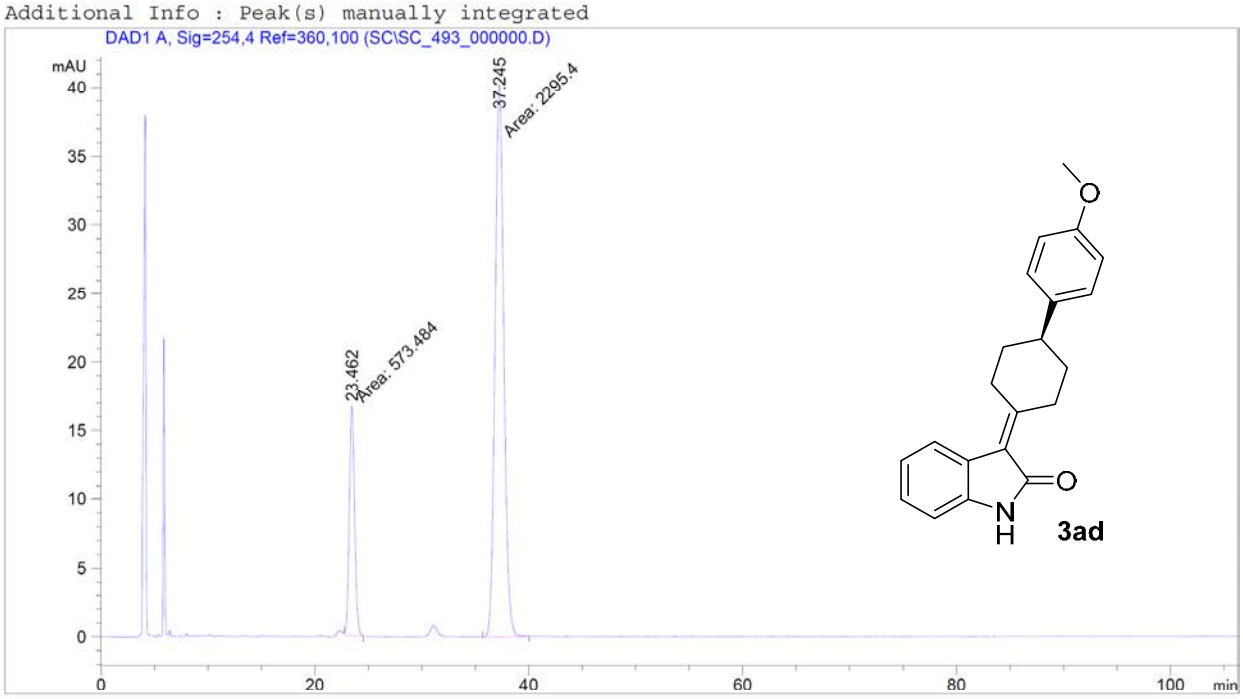

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  23.357 MM    0.5653 5088.33643  150.02054  52.4396
   2  37.062 MM    0.9334 4614.89600   82.40051  47.5604

Totals :                  9703.23242  232.42104


==================================================================
                        *** End of Report ***
```

chiral 10/07/2018 11:32:09 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_493_000000.D
Sample Name: SC_492

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 66
Injection Date   : 21/11/2018 11:42:17
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 21/11/2018 11:40:30 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_493; AD-H 70:30 Hex/IPA; 0.8 ml/min; 25 °C
```

Additional Info : Peak(s) manually integrated

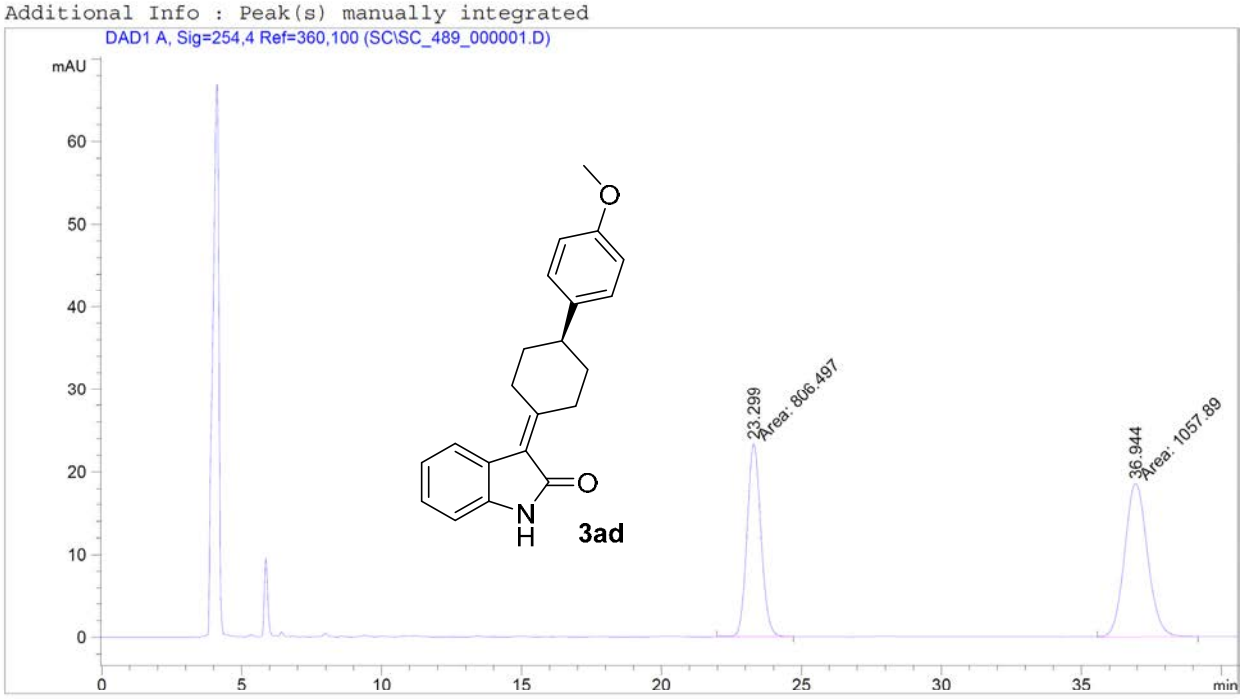



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]    [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  23.462 MM    0.5732  573.48395   16.67565  19.9898
   2  37.245 MM    0.9508 2295.39648   40.23573  80.0102

Totals :                   2868.88043   56.91138


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 12:19:36 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_489_000001.D
Sample Name: SC_489

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 62
Injection Date   : 20/11/2018 18:10:23
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 20/11/2018 18:08:01 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_489; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

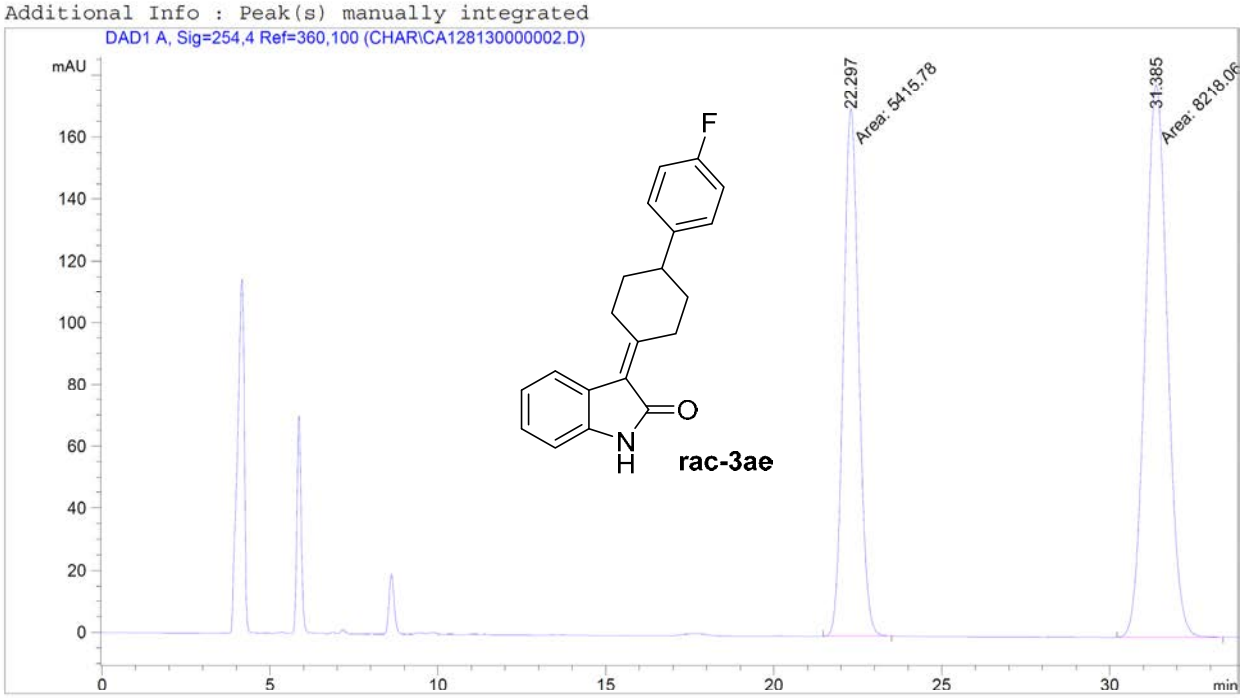



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  23.299 MM    0.5772  806.49738   23.28887  43.2581
   2  36.944 MM    0.9491 1057.88794   18.57702  56.7419

Totals :                  1864.38531   41.86590


==================================================================
                        *** End of Report ***

chiral 12/12/2018 12:21:42 Simone                          Page   1 of 1
```

Data File C:\CHEM32\2\DATA\CHAR\CA128130000002.D
Sample Name: CA_128_130_

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 51
Injection Date   : 13/06/2018 16:30:43
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 13/06/2018 16:01:08 by Luca
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 04/07/2018 11:43:50 by Nico
Sample Info      : CA_128_130_ ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



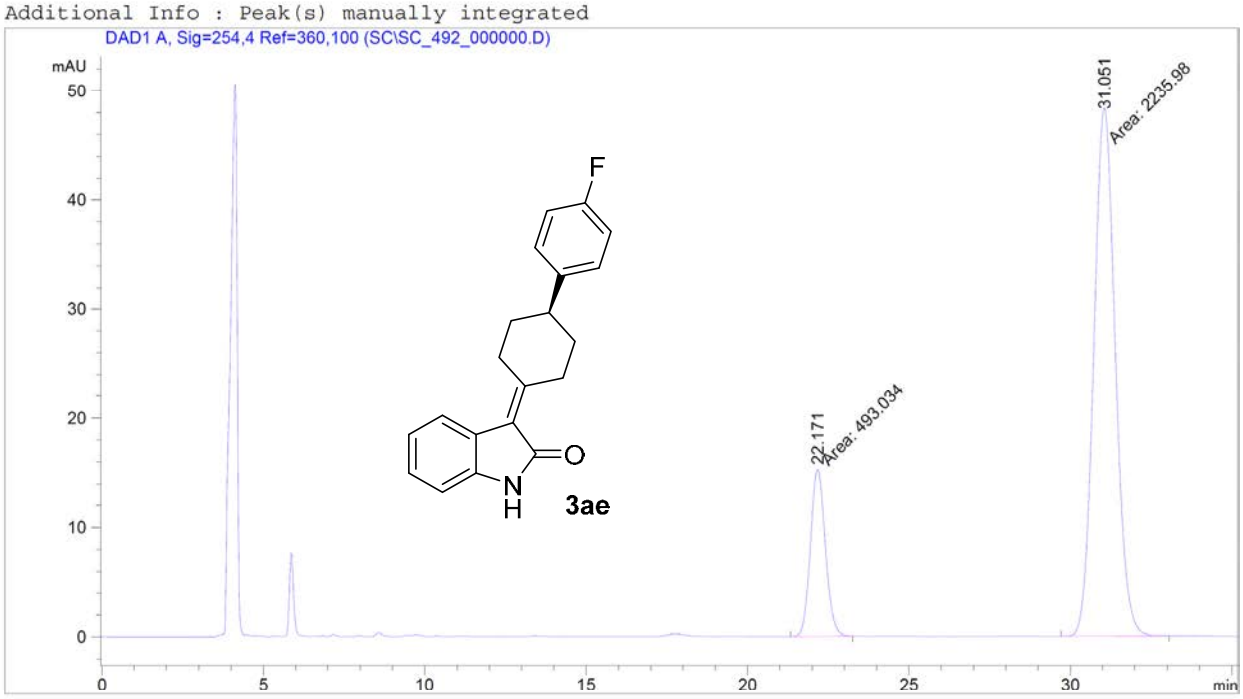

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  22.297 MM    0.5304 5415.77881  170.18056  39.7231
   2  31.385 MM    0.7670 8218.05566  178.58650  60.2769

Totals :                  1.36338e4   348.76706


==================================================================
                        *** End of Report ***
```

chiral 10/07/2018 11:24:11 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_492_000000.D
Sample Name: SC_492

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 65
Injection Date   : 21/11/2018 11:04:57
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 21/11/2018 11:03:22 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_492; AD-H 70:30 Hex/IPA; 0.8 ml/min; 25 °C
```

Additional Info : Peak(s) manually integrated

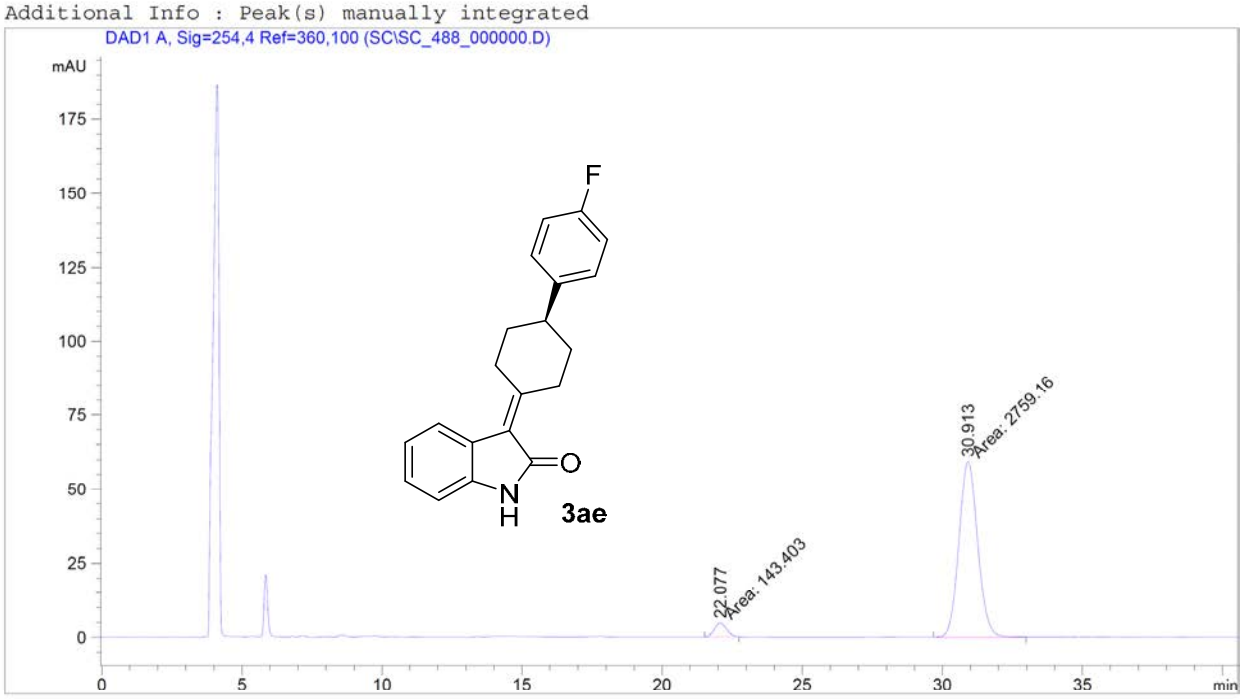



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  22.171 MM    0.5373  493.03406   15.29453  18.0664
   2  31.051 MM    0.7709 2235.98291   48.34072  81.9336

Totals :                  2729.01697   63.63525


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 12:13:46 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_488_000000.D
Sample Name: SC_488

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 61
Injection Date   : 20/11/2018 17:27:05
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 20/11/2018 17:24:27 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/11/2018 09:46:42 by Simone
Sample Info      : SC_488; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

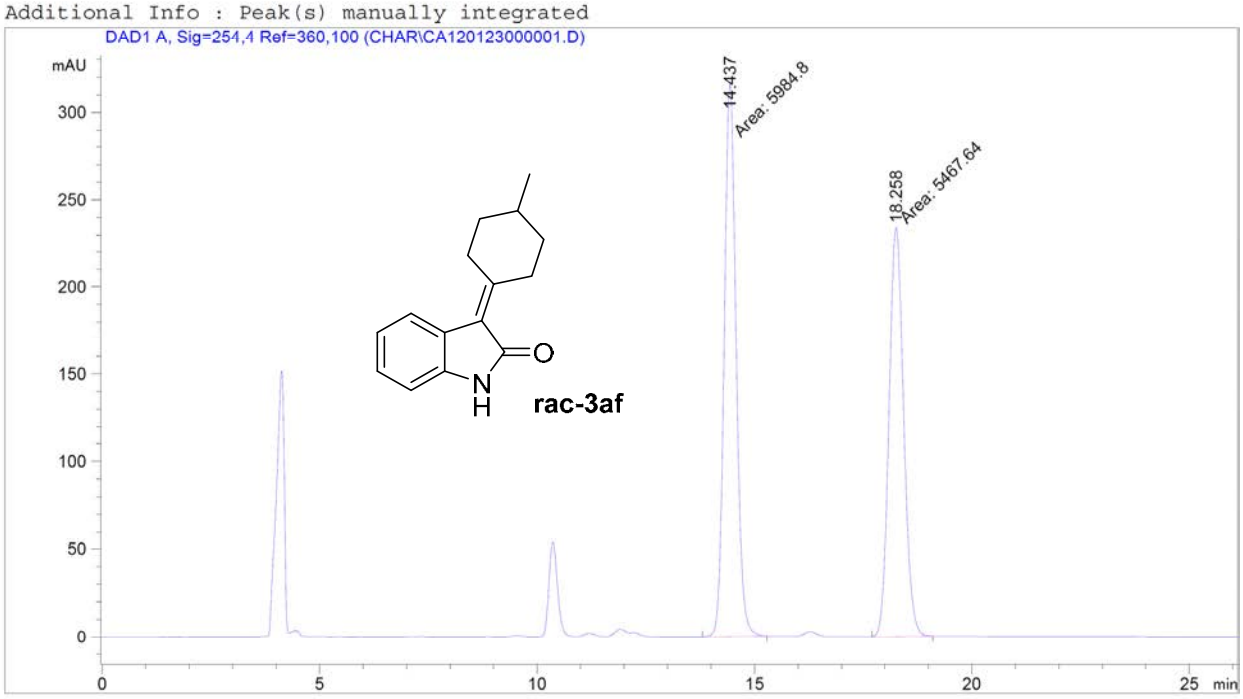



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  22.077 MM    0.5159  143.40326    4.63265   4.9406
   2  30.913 MM    0.7756 2759.16382   59.29223  95.0594

Totals :                  2902.56708   63.92488


==================================================================
                        *** End of Report ***
```

chiral 12/12/2018 12:12:03 Simone Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA120123000001.D
Sample Name: CA_120_123_racemo

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 51
Injection Date   : 06/06/2018 13:15:16
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 06/06/2018 12:48:59 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 10/07/2018 11:34:07 by stefano
                   (modified after loading)
Sample Info      : CA_120_123_racemo ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25
                    gradi


Additional Info : Peak(s) manually integrated
```

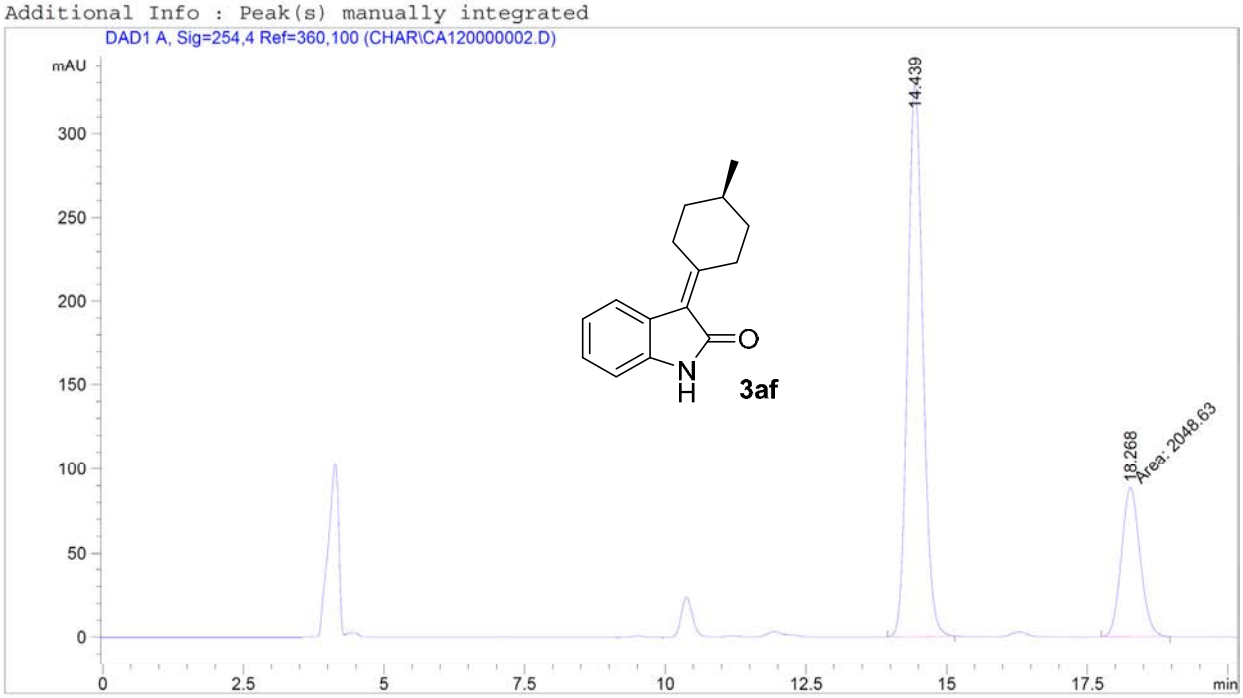



```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.437 MM    0.3156 5984.80078  316.07260  52.2579
   2  18.258 MM    0.3891 5467.63672  234.18680  47.7421

Totals :                  1.14524e4   550.25940
```

Data File C:\CHEM32\2\DATA\CHAR\CA120000002.D
Sample Name: CA_120

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 52
Injection Date   : 06/06/2018 13:43:33
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 06/06/2018 13:41:49 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 10/07/2018 11:34:07 by stefano
                   (modified after loading)
Sample Info      : CA_120 ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated

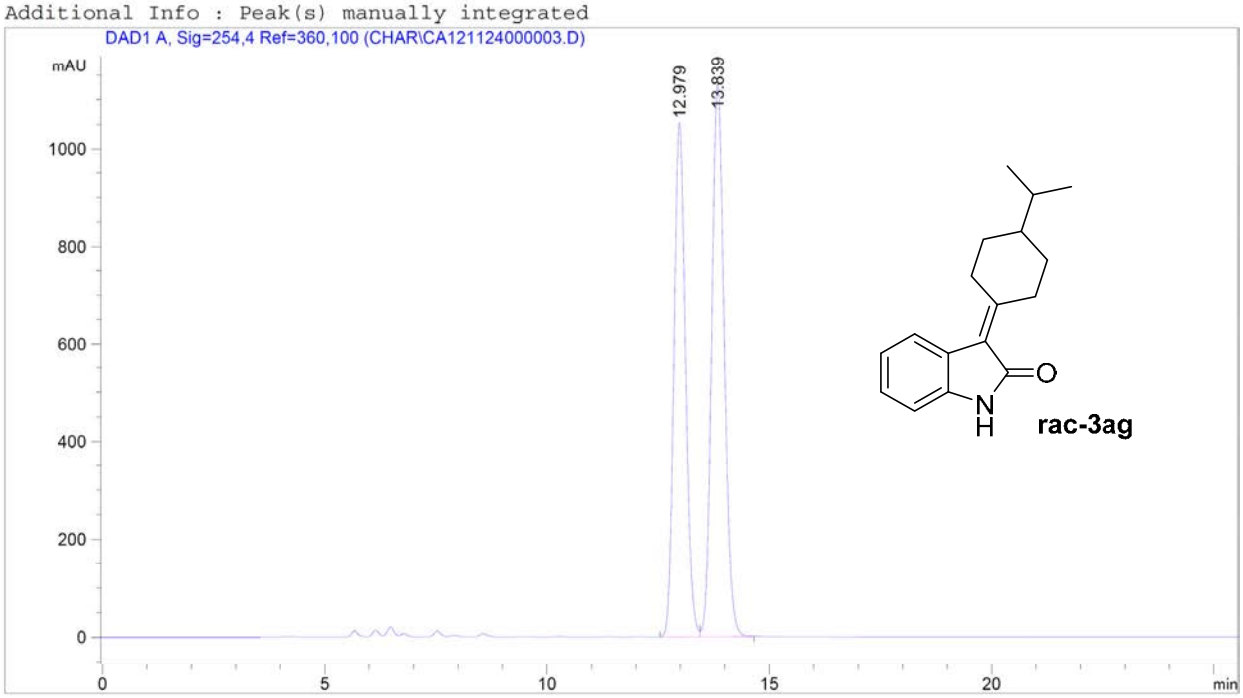



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.439 BB    0.2920 6208.93018  329.26688  75.1908
   2  18.268 MM    0.3854 2048.63208   88.59628  24.8092

Totals :                  8257.56226  417.86316


==================================================================
```

chiral 10/07/2018 11:49:14 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA121124000003.D
Sample Name: CA_121_124

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 1
Injection Date   : 11/07/2018 16:42:10
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 11/07/2018 16:40:27 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 13/07/2018 14:59:51 by Nico
                   (modified after loading)
Sample Info      : CA_121_124; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

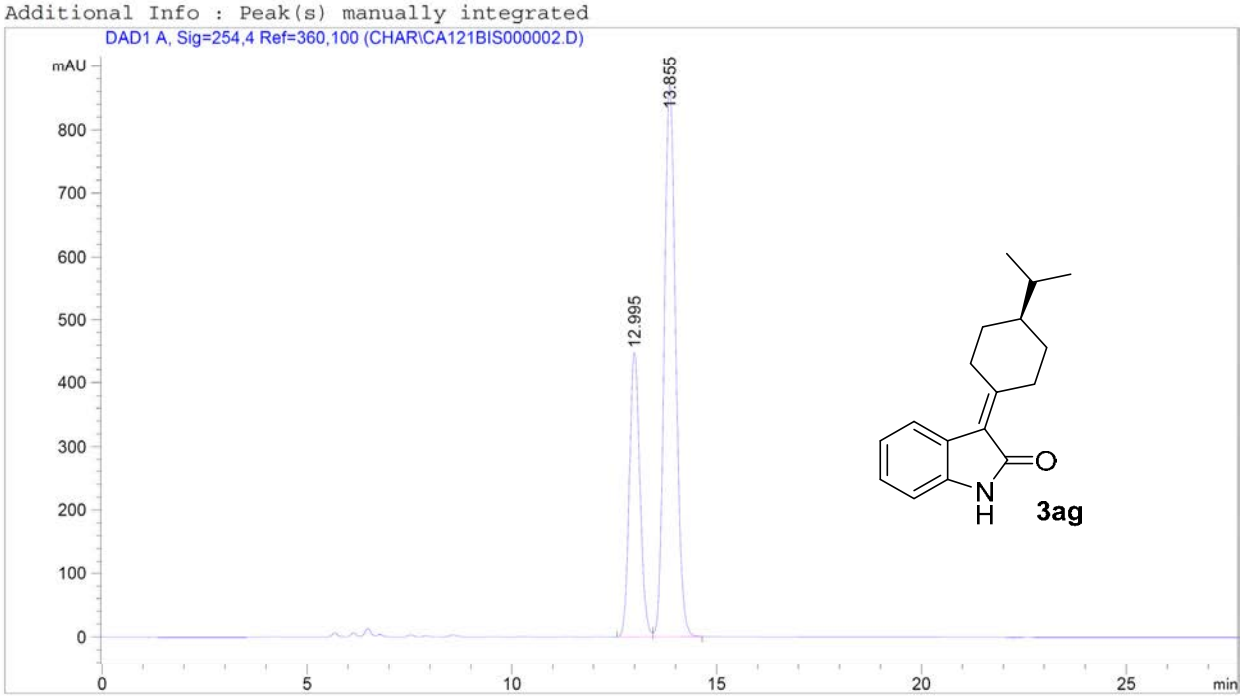



```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  12.979 BV    0.2802 1.89631e4  1052.35205  46.0734
   2  13.839 VB    0.3049 2.21953e4  1131.35315  53.9266

Totals :                  4.11584e4  2183.70520


==================================================================
```

chiral 13/07/2018 15:09:34 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA121BIS000002.D
Sample Name: CA_121_1

```
==========================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 1
Injection Date   : 11/07/2018 16:12:18
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 11/07/2018 16:02:29 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 13/07/2018 14:59:51 by Nico
                   (modified after loading)
Sample Info      : CA_121_1; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi;


Additional Info : Peak(s) manually integrated
```

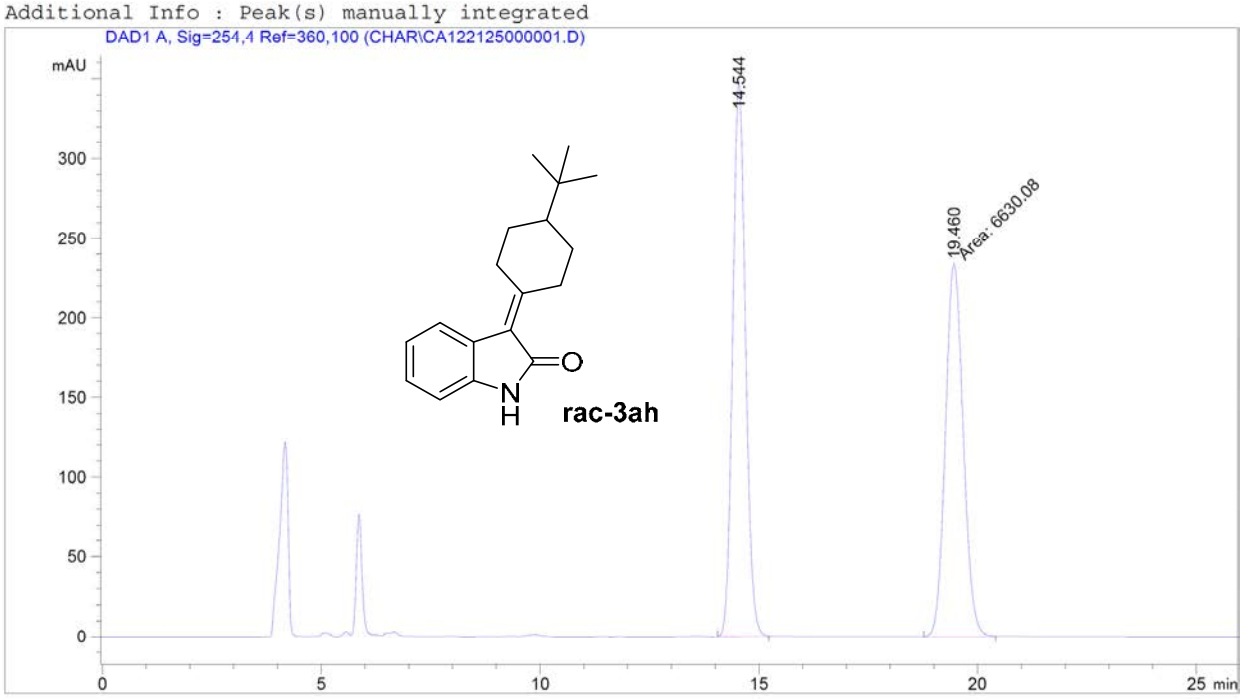



```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  12.995 BV    0.2787 8018.08594  448.12057  32.0403
   2  13.855 VB    0.3037 1.70069e4   871.44598  67.9597

Totals :                  2.50250e4  1319.56656


==========================================================================
```

chiral 13/07/2018 15:10:33 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\CHAR\CA122125000001.D
Sample Name: CA_122_125_racemo

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 57
Injection Date   : 06/06/2018 16:43:45
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 06/06/2018 16:40:39 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 10/07/2018 11:34:07 by stefano
                   (modified after loading)
Sample Info      : CA_122_125_racemo ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25
                    gradi


Additional Info : Peak(s) manually integrated
```

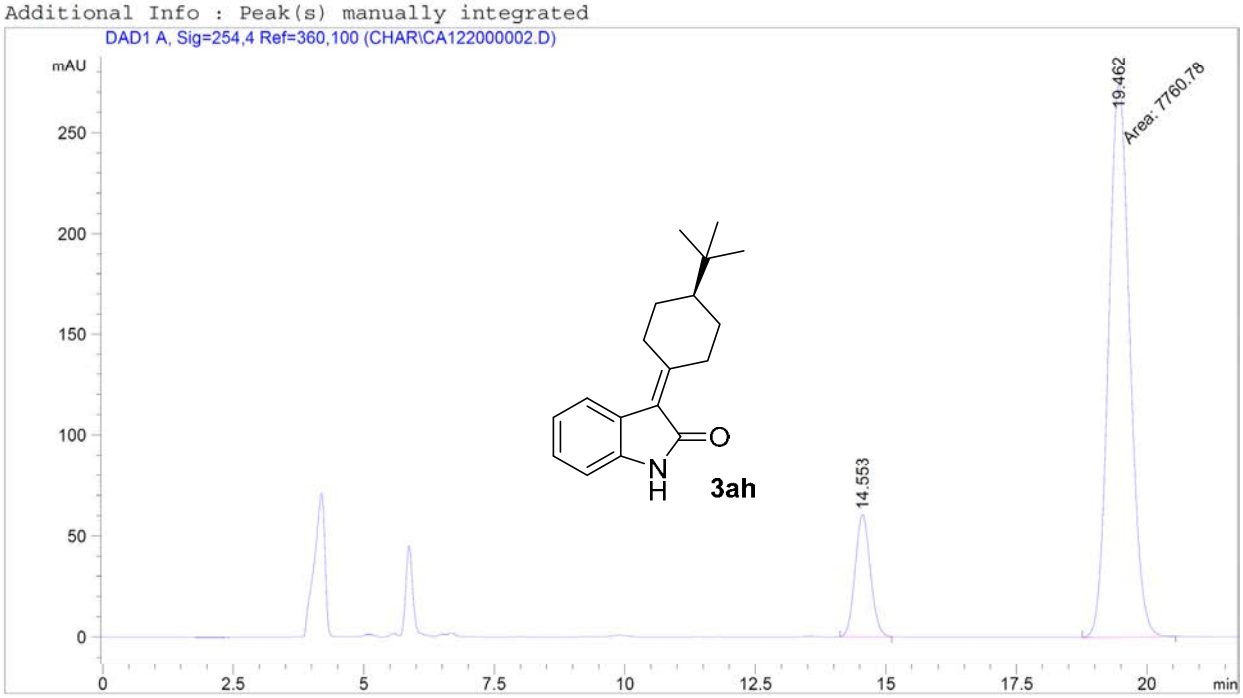



```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.544 BB    0.3162 7077.16797  346.64908  51.6309
   2  19.460 MM    0.4722 6630.07813  233.99960  48.3691

Totals :                  1.37072e4   580.64868
```

Data File C:\CHEM32\2\DATA\CHAR\CA122000002.D
Sample Name: CA_122

```
==================================================================
Acq. Operator    : chiara
Acq. Instrument  : chiral                          Location : Vial 58
Injection Date   : 06/06/2018 17:11:40
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMP.M
Last changed     : 06/06/2018 17:10:06 by chiara
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 10/07/2018 11:34:07 by stefano
                   (modified after loading)
Sample Info      : CA_122 ; AD-H; Hex/IPA 70/30; 0.8 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



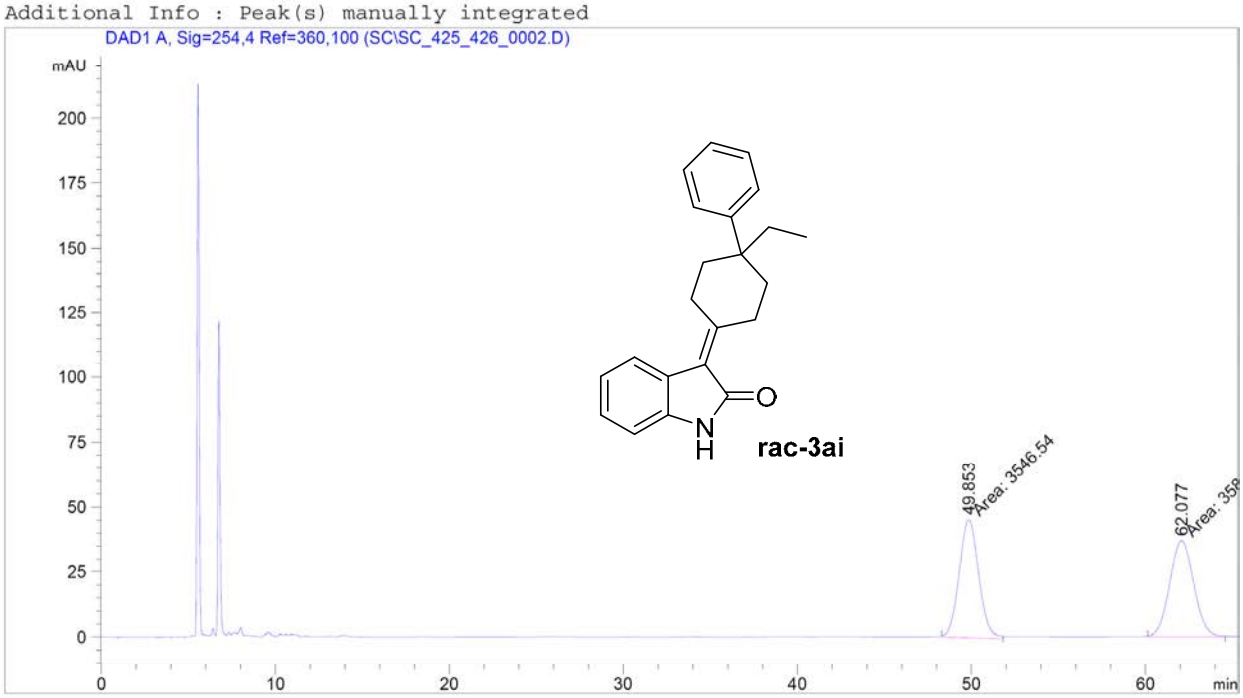

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.553 BB    0.3150 1229.92676   60.53547  13.6800
   2  19.462 MM    0.4720 7760.78223  274.02460  86.3200

Totals :                  8990.70898  334.56007


==================================================================
```

chiral 10/07/2018 12:02:29 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_425_426_0002.D
Sample Name: SC_425_426

```
==================================================================
Acq. Operator    : Simone
Acq. Instrument  : chiral                          Location : Vial 26
Injection Date   : 03/07/2018 15:59:24
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 03/07/2018 15:03:51 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 13/07/2018 14:59:51 by Nico
                   (modified after loading)
Sample Info      : SC_425_426; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated

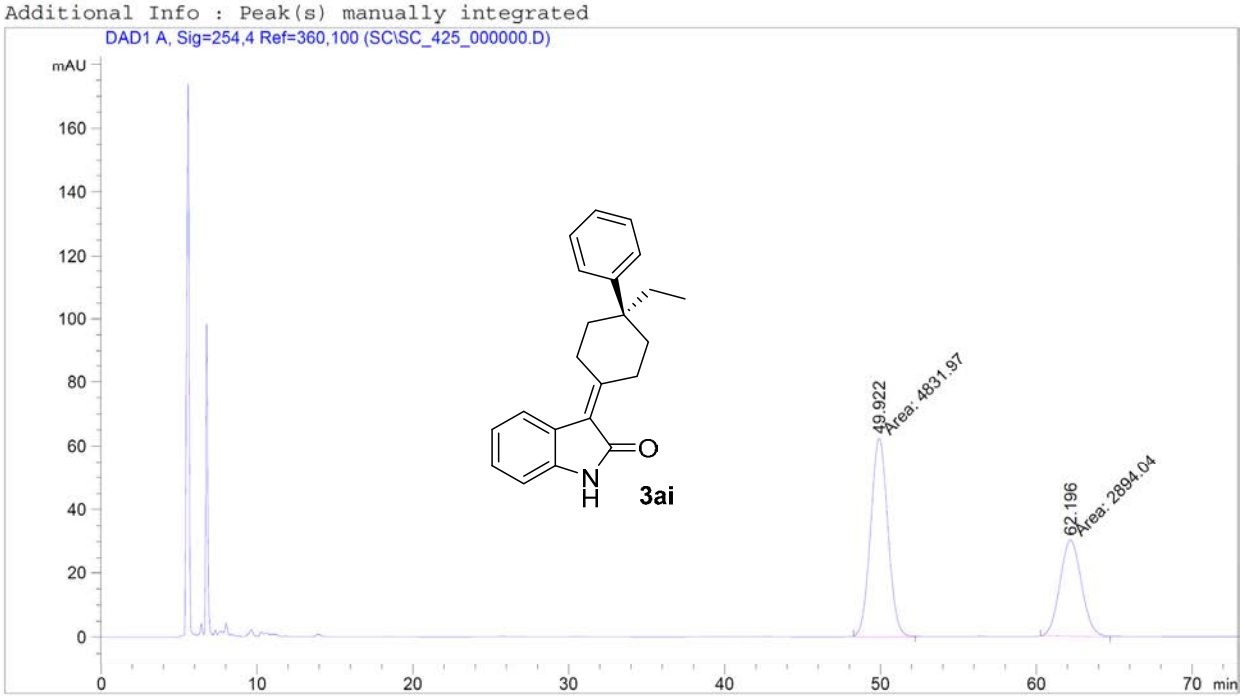



```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  49.853 MM    1.3001 3546.54028   45.46668  49.7033
   2  62.077 MM    1.6094 3588.88110   37.16628  50.2967

Totals :                  7135.42139   82.63296


==================================================================
```

chiral 13/07/2018 14:59:55 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\SC\SC_425_000000.D
Sample Name: SC_425

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 25
Injection Date   : 03/07/2018 18:19:06
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 03/07/2018 18:17:32 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 13/07/2018 14:59:51 by Nico
                   (modified after loading)
Sample Info      : SC_425; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi


Additional Info : Peak(s) manually integrated
```

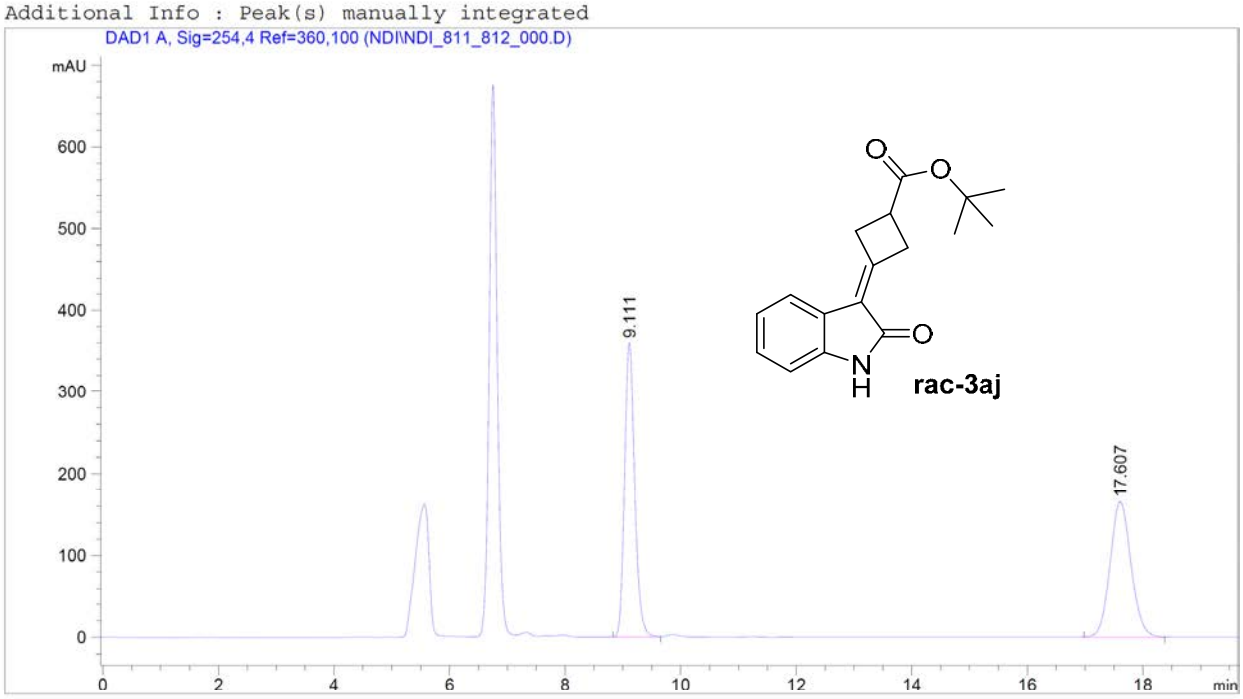



```
==================================================================
                          Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  49.922 MM    1.2901 4831.96582   62.42515  62.5416
   2  62.196 MM    1.5968 2894.04077   30.20658  37.4584

Totals :                  7726.00659   92.63173


==================================================================
```

chiral 13/07/2018 15:01:05 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_811_812_000.D
Sample Name: NDI_811_812

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 10
Injection Date   : 03/07/2018 17:06:40
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 03/07/2018 17:05:05 by Simone
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/06/2018 17:26:24 by Luca
Sample Info      : NDI_811_812; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi

Additional Info : Peak(s) manually integrated
```



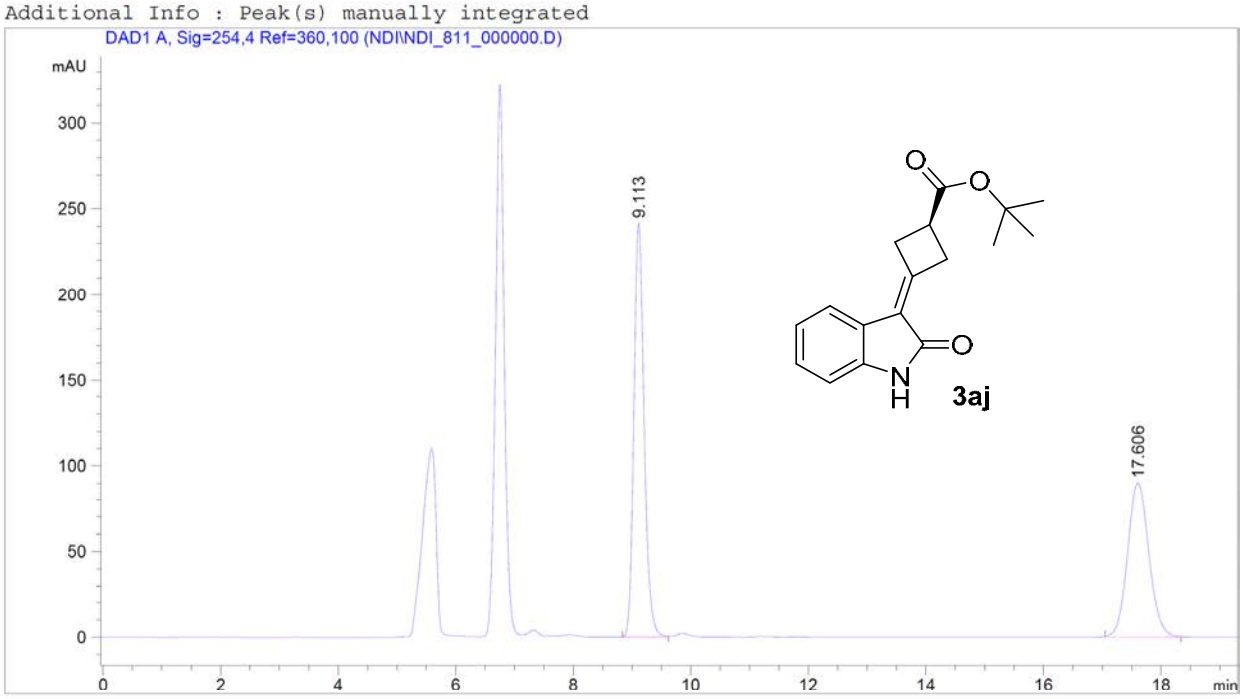

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   9.111 BB    0.1862 4383.91553  359.74213  51.2259
   2  17.607 BB    0.3909 4174.08398  165.12599  48.7741

Totals :                  8557.99951  524.86812


==================================================================
                          *** End of Report ***
```

chiral 03/07/2018 17:27:28 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_811_000000.D
Sample Name: NDI_811

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 11
Injection Date   : 03/07/2018 17:28:17
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 03/07/2018 17:26:44 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 29/06/2018 17:26:24 by Luca
Sample Info      : NDI_811; AD-H; Hex/IPA 50/50; 0.6 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



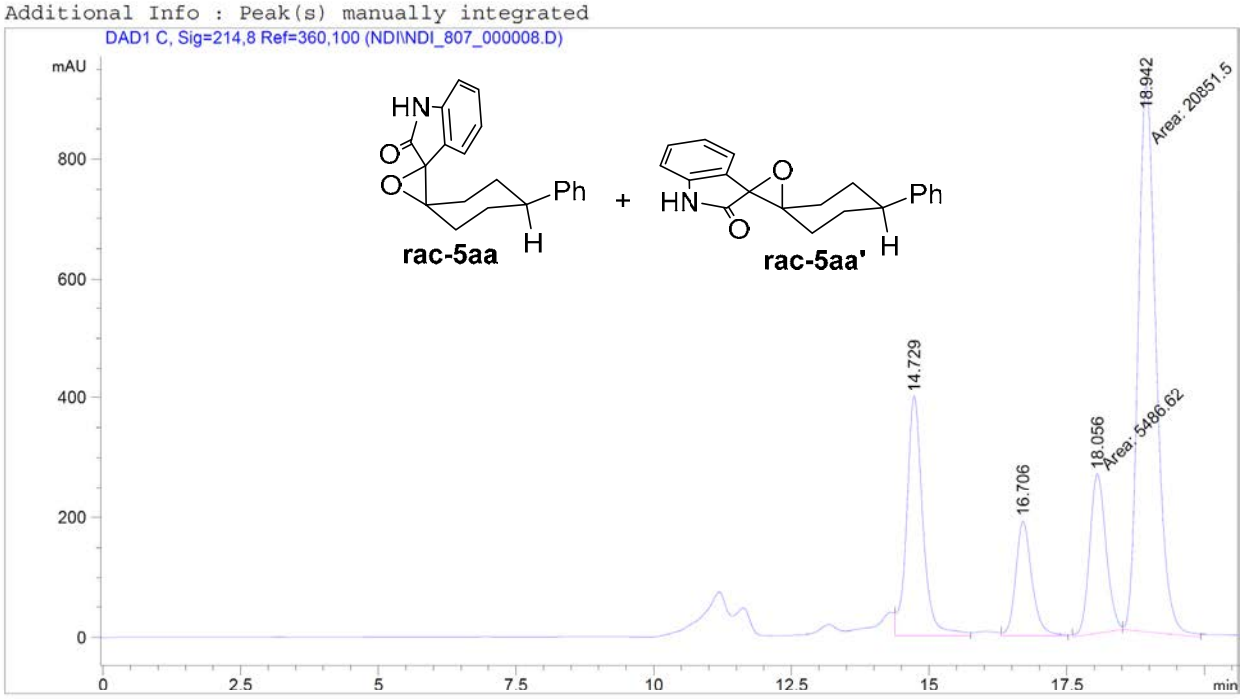

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   9.113 BB    0.1872 2923.85913  241.63232  56.2887
   2  17.606 BB    0.3921 2270.53882   90.06987  43.7113

Totals :                  5194.39795  331.70219


==================================================================
                        *** End of Report ***
```

chiral 03/07/2018 17:49:54 stefano Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_807_000008.D
Sample Name: NDI_807

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 7
Injection Date   : 27/06/2018 14:16:26
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 27/06/2018 13:52:21 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 22/06/2018 09:04:12 by stefano
Sample Info      : NDI_807; AD-H; Hex/IPA 40/60; 0.3 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 C, Sig=214,8 Ref=360,100
```

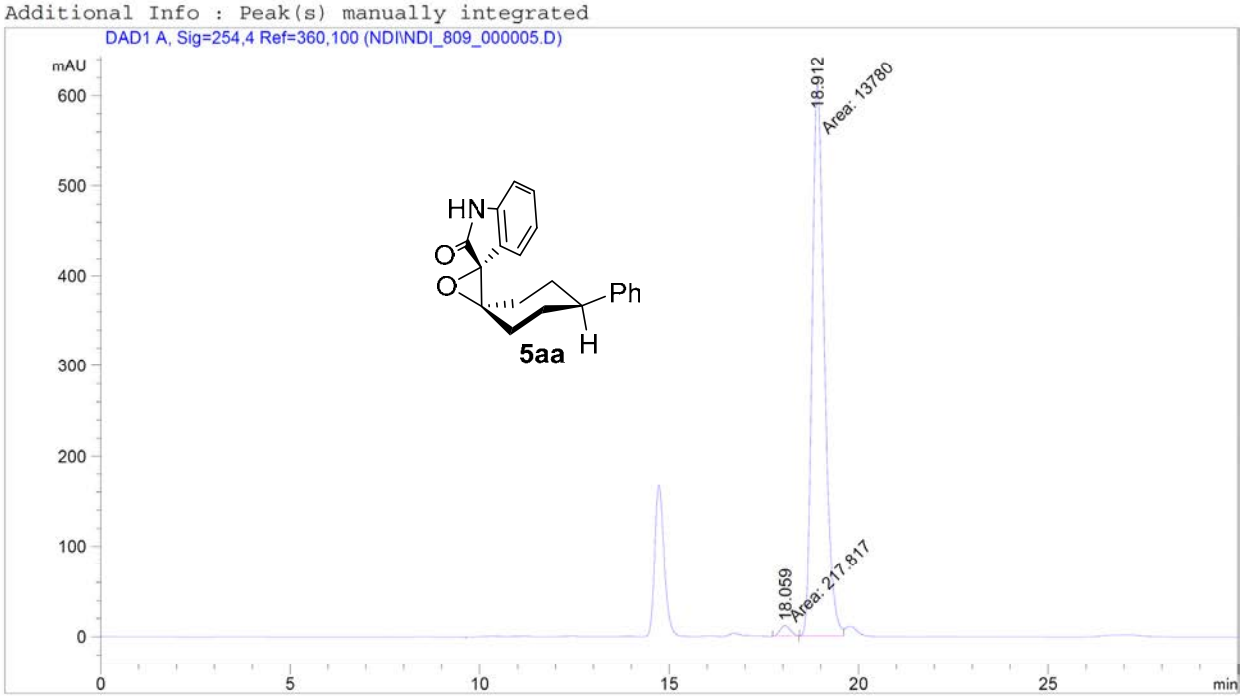
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	14.729	VB	0.3028	8098.08447	399.03406	21.1399
2	16.706	VB	0.3070	3870.95239	190.52986	10.1050
3	18.056	MM	0.3433	5486.61523	266.36639	14.3227
4	18.942	MM	0.3798	2.08515e4	914.94312	54.4324

Totals : 3.83072e4 1770.87343

Data File C:\CHEM32\2\DATA\NDI\NDI_809_000005.D
Sample Name: NDI_809

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 9
Injection Date   : 27/06/2018 14:39:03
                                                  Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 27/06/2018 14:37:24 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 27/06/2018 16:19:42 by Nico
                   (modified after loading)
Sample Info      : NDI_809; AD-H; Hex/IPA 40/60; 0.3 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated



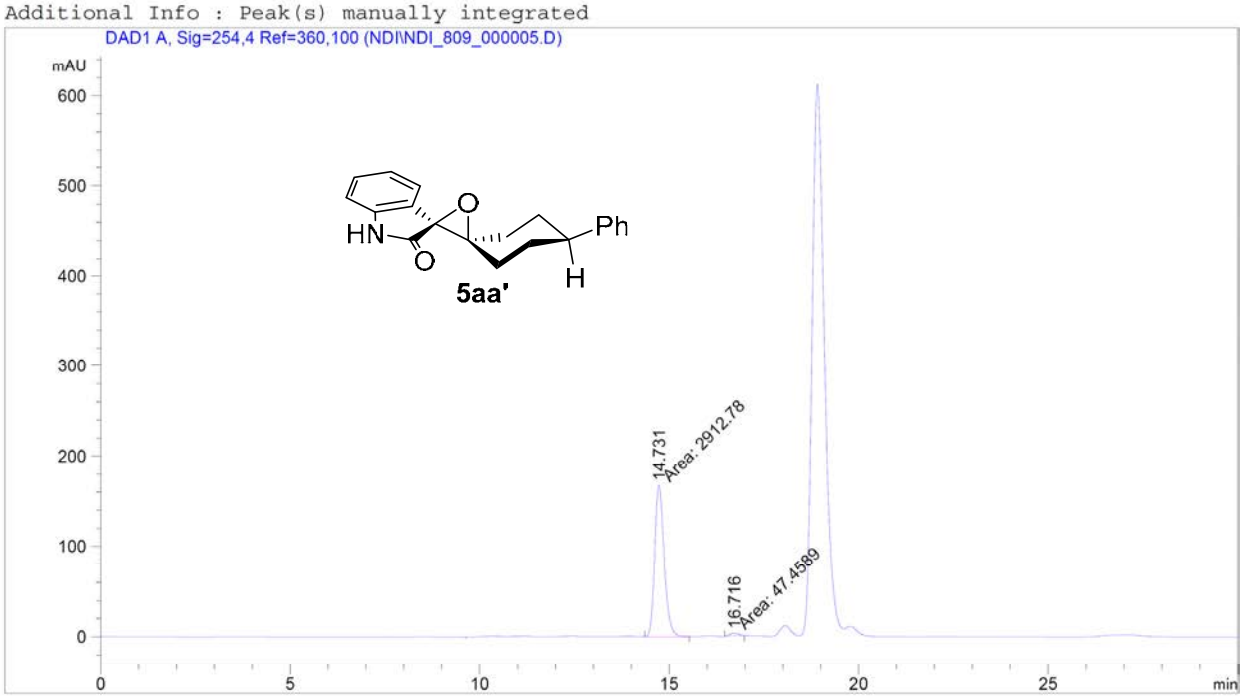

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1  18.059 MM    0.3133  217.81723   11.58815   1.5561
   2  18.912 MF    0.3751 1.37800e4   612.28418  98.4439

Totals :                  1.39979e4   623.87233


==================================================================
```

chiral 27/06/2018 16:19:45 Nico Page 1 of 1

Data File C:\CHEM32\2\DATA\NDI\NDI_809_000005.D
Sample Name: NDI_809

```
==================================================================
Acq. Operator    : Nico
Acq. Instrument  : chiral                          Location : Vial 9
Injection Date   : 27/06/2018 14:39:03
                                                 Inj Volume : 10.0 µl
Acq. Method      : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 27/06/2018 14:37:24 by Nico
                   (modified after loading)
Analysis Method  : C:\CHEM32\2\METHODS\TMPFULL.M
Last changed     : 27/06/2018 16:16:00 by Nico
                   (modified after loading)
Sample Info      : NDI_809; AD-H; Hex/IPA 40/60; 0.3 ml/min; 25 gradi
```

Additional Info : Peak(s) manually integrated




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1  14.731 MM    0.2905 2912.78174  167.11813  98.3968
   2  16.716 MM    0.2716   47.45889    2.91233   1.6032

Totals :                  2960.24063  170.03046


==================================================================
```

chiral 27/06/2018 16:16:37 Nico Page 1 of 1