Supporting information

Diastereoselective synthesis and structure-affinity relationships of σ_1 receptor ligands with spirocyclic scaffold

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Contents

Chemistry, General Methods

Oxygen and moisture sensitive reactions were carried out under nitrogen, dried with silica gel with moisture indicator (orange gel, VWR, Darmstadt, Germany) and in dry glassware (Schlenk flask or Schlenk tube). Temperature was controlled with dry ice/acetone (-78 °C), ice/water (0 °C), Cryostat (Julabo TC100E-F, Seelbach, Germany), magnetic stirrer MR 3001 K (Heidolph, Schwalbach, Germany) or RCT CL (IKA, Staufen, Germany), together with temperature controller EKT HeiCon (Heidolph) or VT-5 (VWR) and PEG or silicone bath. All solvents were of analytical or technical grade quality. Demineralized water was used. CH_2Cl_2 was distilled from CaH_2; THF was distilled from sodium/benzophenone; MeOH was distilled from magnesium methanolate. Thin layer chromatography (tlc): tlc silica gel 60 F_{254} on aluminum sheets (VWR). Flash chromatography (fc): Silica gel 60, 40–63 µm (VWR); parentheses include: diameter of the column (ø), length of the stationary phase (h), fraction size (v) and eluent. Automated flash chromatography: Isolera™ Spektra One (Biotage®); parentheses include: cartridge size, eluent, fractions size was always 20 mL. Dry column vacuum chromatography (DCVC) was performed according to Pedersen *et al* using glass funnels with sintered glass disc filters and a height of 11 cm;[1] parentheses include: diameter of the column (ø), length of the compressed stationary phase (h), eluent. Melting point: Melting point system MP50 (Mettler Toledo, Gießen, Germany), open capillary, uncorrected. MS: MicroTOFQII mass spectrometer (Bruker Daltonics, Bremen, Germany); deviations of the found exact masses from the calculated exact masses were 5 ppm or less; the data were analyzed with DataAnalysis® (Bruker Daltonics). NMR: NMR spectra were recorded in deuterated solvents on Agilent DD2 400 MHz and 600 MHz spectrometers (Agilent, Santa Clara CA, USA); chemical shifts (δ) are reported in parts per million (ppm) against the reference substance tetramethylsilane and calculated using the solvent residual peak of the undeuterated solvent; coupling constants are given with 0.5 Hz resolution; assignment of ^{1}H and ^{13}C NMR signals was supported by 2-D NMR techniques where necessary. IR: FT/IR IR Affinity®-1 spectrometer (Shimadzu, Düsseldorf, Germany) using ATR technique. Purity by quantitative NMR (qNMR) was performed according to literature using 1,3,5-trimethoxybenzene (Sigma-Aldrich, standard for quantitative NMR, TraceCERT®) as the standard.[2]

HPLC Analysis

Set 1: Pump: LPG-3400SD, degasser: DG-1210, autosampler: ACC-3000T, UV-detector: VWD-3400RS, interface: DIONEX UltiMate 3000, data acquisition: Chromeleon 7 (Thermo Fisher Scientific).

Set 2: pump: L-7150A, autosampler: L-7200, UV-detector: L-7400, interface: D-7000 I/F, data acquisition: HSM-software (all LaChrom, Merck Hitachi).

Method 1 (Purity)

Set 1

Column:	LiChropher® 60 RP-select B (5 µm), LiChroCART® 250-4 mm cartridge
Guard column:	LiChropher® 60 RP-select B (5 µm), LiChroCART® 4-4 mm cartridge (No.: 1.50963.0001), manu-CART® NT cartridge holder
Flow rate:	1.0 mL/min
Injection volume:	5.0 µL; method: cut lead and rear
Detection wavelength	210 nm
Solvent A:	Demineralized water + 0.05 % (V/V) trifluoroacetic acid
Solvent B:	Acetonitrile with 0.05 % (V/V) trifluoroacetic acid
Gradient elution (% A):	0 - 4 min: 90 %; 4 - 29 min: gradient from 90 % to 0 %; 29 - 31 min: 0 %; 31 - 31.5 min: gradient from 0 % to 90 %; 31.5 - 40 min: 90 %.

Method 2 (preparative separation)

Set 2

Column:	Agilent Prep-C18 (10 µm), 21.2 x 250 mm
Flow rate	20 mL/min
Injection Volume	400 µL, Method: Full
Detection Wavelength	210 nm
Run time	30 min
Solvent	Acetonitrile:H_2O: 50:50

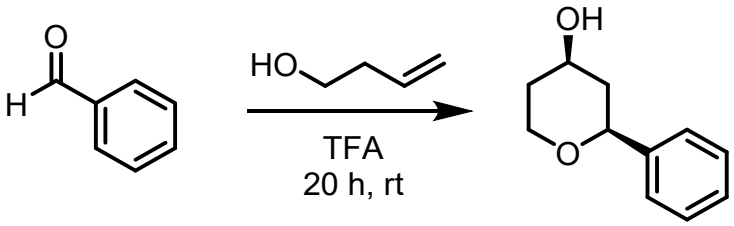
Method 3 (preparative separation)

Set 2

Column:	Agilent Prep-C18 (10 µm), 21.2 x 250 mm
Guard Column	-
Flow rate	20 mL/min
Injection Volume	400 µL, Method: Full
Detection Wavelength	210 nm
Run time	30 min
Solvent	Acetonitrile:H_2O: 40:60

Synthesis of some educts

cis-2-Phenyltetrahydro-2*H*-pyran-4-ol



At room temperature under N_2, trifluoracetic acid (59.4 mL, 777 mmol, 10.0 eq.) was added to a mixture of benzaldehyde (7.92 mL, 77.7 mmol, 1.00 eq.) and but-3-en-1-ol (10.0 mL, 116 mmol, 1.50 eq.). The reaction mixture was stirred for 20 h at room temperature. Saturated aqueous Na_2CO_3 solution (250 mL) followed by NaOH (4.00 g) was added to the mixture and the solution was stirred for 72 h at room temperature. The aqueous layer was extracted with CH_2Cl_2 (4 x 150 mL) and the combined organic layers were washed with water, brine and dried (Na_2SO_4). The organic layer was concentrated *in vacuo* and the residue was purified by DCVC (Ø = 6 cm, h = 5 cm, cHex:EtOAc: 85:15 → 50:50).

Yellow oil, R_f = 0.20 (cHex/EtOAc 80:20), yield 12.1 g (87%).

$C_{11}H_{14}O_2$ (178.2 g/mol).

Analytical data in accordance with literature.[3]

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 1.55 (dt, J = 12.6/11.2 Hz, 1H, 3-C$H_{2(ax)}$), 1.63 (tdd, J = 12.6/11.0/4.9 Hz, 1H, 5-C$H_{2(ax)}$), 1.96 (ddq, J = 12.5/4.2/2.0 Hz, 1H, 5-C$H_{2(eq)}$), 2.18 (ddt, J = 12.5/4.4/2.2 Hz, 1H, 3-C$H_{2(eq)}$), 3.58 (ddd, J = 12.6/11.9/2.1 Hz, 1H, 6-C$H_{2(ax)}$), 3.93 (tt, J = 11.0/4.6 Hz, 1H, 4-C*H*), 4.17 (ddd, J = 11.8/4.9/1.8 Hz, 1H, 6-C$H_{2(eq)}$), 4.31 (dd, J = 11.4/2.1 Hz, 1H, 2-C*H*), 7.25 – 7.29 (m, 1H, 4-$H_{(Ph)}$), 7.32 – 7.36 (m, 4H, 2-$H_{(Ph)}$, 3-$H_{(Ph)}$, 5-$H_{(Ph)}$, 6-$H_{(Ph)}$). A signal for the OH proton is not observed in the spectrum.

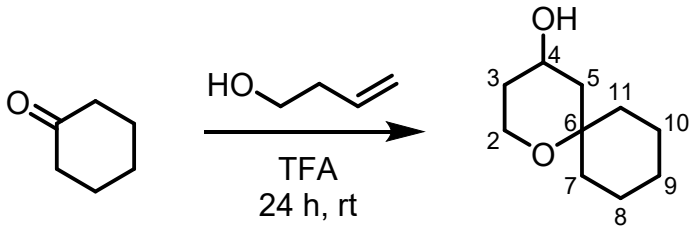
^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) = 35.6 (*C*-5), 43.4 (*C*-3), 66.5 (*C*-6), 68.6 (*C*-4), 78.5 (*C*-2), 126.0 (*C*-$2_{(Ph)}$, *C*-$6_{(Ph)}$), 127.8 (*C*-$4_{(Ph)}$), 128.6 (*C*-$3_{(Ph)}$, *C*-$5_{(Ph)}$), 142.0 (*C*-$1_{(Ph)}$).

HRMS: m/z = 171.1374, calcd. 171.1380 for $C_{11}H_{15}O_2^+$ $[M+H]^+$.

IR (neat): $\tilde{\nu}$ [cm^{-1}] = 3348 (O-H),3028 (C-H_{aryl}), 2941 (CH_{alkyl}).

Purity (HPLC): 96.3% (t_R = 12.7 min).

(*RS*)-1-Oxaspiro[5.5]undecan-4-ol



At room temperature under N_2, trifluoracetic acid (29.7 mL, 388 mmol, 10.0 eq.) was added to a mixture of cyclohexanone (4.02 mL, 38.8 mmol, 1.00 eq.) and but-3-en-1-ol (5.00 mL, 58.3 mmol, 1.50 eq.). The reaction mixture was stirred for 24 h at room temperature. Saturated aqueous Na_2CO_3 solution (120 mL) followed by NaOH (4.00 g) was added to the mixture and the solution was stirred for 72 h at room temperature. The aqueous layer was extracted with CH_2Cl_2 (4 x 150 mL) and the combined organic layers were washed with water, brine and dried (Na_2SO_4). The organic layer was concentrated *in vacuo* and the residue was purified by DCVC (Ø = 6 cm, h = 5 cm, cHex:EtOAc: 85:15 → 50:50).

$C_{10}H_{18}O_2$ 170.3 (g/mol).

Yellow oil, R_f = 0.23 (cHex/EtOAc 80:20), yield 3.73 g (56%).

Analytical data in accordance with literature.[4]

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.19 (dd, J = 12.7/10.8 Hz, 1H, 5-C$H_{2(ax)}$), 1.25 – 1.31 (m, 1H, 9-C$H_{2(ax)}$), 1.31 – 1.36 (m, 1H, 7/11-C$H_{2(ax)}$), 1.36 – 1.42 (m, 2H, 7/11-C$H_{2(eq)}$, 8/10-C$H_{2(ax)}$), 1.43 – 1.48 (m, 2H, 3-C$H_{2(ax)}$, 8/10-C$H_{2(ax)}$), 1.49 – 1.55 (m, 2H, 8/10-C$H_{2(eq)}$, 9-C$H_{2(eq)}$), 1.57 – 1.63 (m, 1H, 7/11-C$H_{2(ax)}$), 1.63 – 1.70 (m, 1H, 8/10-C$H_{2(eq)}$), 1.81 – 1.87 (m, 1H, 7/11-C$H_{2(eq)}$), 1.86 – 1.95 (m, 2H, 3-C$H_{2(eq)}$, 5-C$H_{2(eq)}$), 3.58 (td, J = 12.1/2.4 Hz, 1H, 2-C$H_{2(ax)}$), 3.79 (ddd, J = 12.1/5.2/2.4 Hz, 1H, 2-C$H_{2(eq)}$), 3.90 – 4.02 (m, 1H, 4-CH). A signal for the OH proton is not observed in the spectrum.

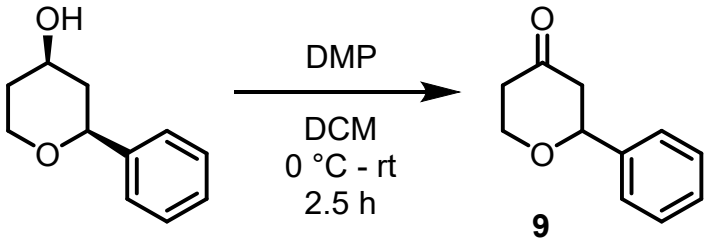
^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) = 21.6 (*C*-8/10), 21.9 (*C*-8/10), 26.2 (*C*-9), 31.3 (*C*-7/11), 36.1 (*C*-3), 39.8 (*C*-7/11), 45.2 (*C*-5), 59.2 (*C*-2), 65.0 (*C*-4), 73.8 (*C*-6).

HRMS: m/z = 171.1374, calcd. 171.1380 for $C_{10}H_{19}O_2^+$ $[M+H]^+$.

IR (neat): $\tilde{\nu}$ [cm^{-1}] = 3356 (O-H), 2930 (CH_{alkyl}).

Purity (qNMR): 95.4%.

(*RS*)-2-Phenyltetrahydropyran-4-one (9)



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At 0 °C under N_2, Dess-Martin periodinane (DMP, 13.1 g, 30.9 mmol, 1.10 eq.) was added portionwise to a solution of *cis*-2-phenyltetrahydro-2*H*-pyran-4-ol (5.00 g, 28.1 mmol, 1.00 eq.) in CH_2Cl_2 (60 mL). The reaction mixture was stirred for 2.5 h while slowly warming up to room temperature. Saturated aqueous Na_2SO_3 solution (30 mL) and saturated aqueous Na_2CO_3 (30 mL) were added and the suspension was filtered. The filtrate was extracted with CH_2Cl_2 (3 x 100 mL). The combined organic layers were washed with aqueous Na_2CO_3 solution, water and brine and dried (Na_2SO_4). The organic layer was concentrated *in vacuo* and the residue was purified by DCVC (Ø = 6 cm, h = 5 cm, cHex/EtOAc: 100:0 → 60:40).

Colorless oil, R_f =0.41 (cHex/EtOAc 75:25), yield 3.90 g (79%).

$C_{11}H_{12}O_2$ (176.2 g/mol).

Analytical data in accordance with literature.[5]

^{1}H NMR (600 MHz, $CDCl_3$): δ (ppm) = 2.44 (ddt, *J* = 14.8/2.9/1.6 Hz, 1H, 5-C$H_{2(eq)}$), 2.63 – 2.68 (m, 2H, 3-CH_2), 2.73 (ddd, *J* = 14.7/12.3/7.4 Hz, 1H, 5-C$H_{2(ax)}$), 3.85 (ddd, *J* = 12.4/11.6/2.9 Hz, 1H, 6-C$H_{2(ax)}$), 4.44 (ddd, *J* = 11.6/7.4/1.6 Hz, 1H, 6-C$H_{2(eq)}$), 4.65 (dd, *J* = 8.8/5.4 Hz, 1H, 2-C*H*), 7.29 – 7.34 (m, 1H, 4-$H_{(Ph)}$), 7.35 – 7.41 (m, 4H, 2-$H_{(Ph)}$, 3-$H_{(Ph)}$, 5-$H_{(Ph)}$, 6-$H_{(Ph)}$).

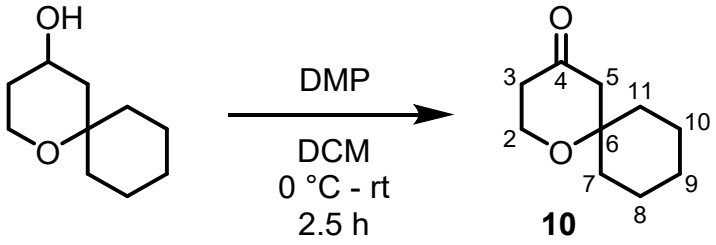
^{13}C NMR (151 MHz, $CDCl_3$): δ (ppm) = 42.3 (*C*-5), 50.1 (*C*-3), 66.9 (*C*-6), 80.0 (*C*-2), 125.8 (*C*-$2_{(Ph)}$, *C*-$6_{(Ph)}$), 128.3 (*C*-$4_{(Ph)}$), 128.8 (*C*-$3_{(Ph)}$, *C*-$5_{(Ph)}$), 140.7 (*C*-$1_{(Ph)}$), 206.5 (*C*-4).

HRMS: m/z = 177.0910, calcd. 177.0910 for $C_{11}H_{13}O_2^+$ $[M+H]^+$.

IR (neat): $\tilde{\nu}$ [cm^{-1}] = 3024 (C-H_{aryl}), 2968 (CH_{alkyl}), 1717 (C=O).

Purity (HPLC): 96.0% (t_R = 14.9 min).

1-Oxaspiro[5.5]undecan-4-one (10)



At 0 °C under N_2, Dess-Martin periodinane (DMP, 7.81 g, 18.4 mmol, 1.10 eq.) was added portionwise to a solution of (*RS*)-1-oxaspiro[5.5]undecan-4-ol (2.85 g, 16.7 mmol, 1.00 eq.) in CH_2Cl_2 (40 mL). The reaction mixture was stirred for 3 h while slowly warming up to room temperature. A few drops of water were added and the suspension was filtered off. The filtrate was washed with water (3 x 30 mL), brine and dried (Na_2SO_4). The organic layer was concentrated *in vacuo* and the residue was purified by DCVC (Ø = 4 cm, h = 5 cm, cHex/EtoAc: 100:0 → 60:40).

Colorless oil, R_f = 0.50 (cHex/EtOAc 75:25), yield 2.50 g (89%).

$C_{10}H_{16}O_2$ (168.2 g/mol).

Analytical data in accordance with literature.[6]

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = 1.20 – 1.29 (m, 1H, 9-C$H_{2(ax)}$), 1.30 – 1.39 (m, 2H, 7-C$H_{2(ax)}$, 11-C$H_{2(ax)}$), 1.39 – 1.49 (m, 2H, 8-C$H_{2(ax)}$, 10-C$H_{2(ax)}$), 1.49 – 1.65 (m, 3H, 8-C$H_{2(eq)}$, 9-C$H_{2(eq)}$, 10-C$H_{2(eq)}$), 1.69 – 1.78 (m, 2H, 7-C$H_{2(eq)}$, 11-C$H_{2(eq)}$), 2.30 – 2.33 (m, 2H, 5-CH_2), 2.37 – 2.45 (m, 2H, 3-CH_2), 3.96 (t, J = 6.1 Hz, 2H, 2-CH_2).

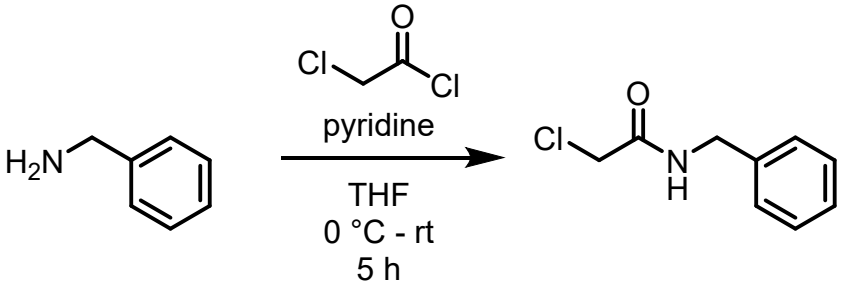
^{13}C NMR (101 MHz, $CDCl_3$): δ (ppm) = 21.4 (*C*-8, *C*-10), 25.5 (*C*-9), 35.3 (*C*-7, *C*-11), 42.0 (*C*-3), 53.2 (*C*-5), 60.1 (*C*-2), 76.8 (*C*-6), 208.0 (*C*-4).

HRMS: m/z = 169.1223, calcd. 169.1223 for $C_{10}H_{17}O_2^+$ $[M+H]^+$.

IR (neat): $\tilde{\nu}$ [cm^{-1}] = 2930 (CH_{alkyl}), 1715 (C=O).

Purity (qNMR): 99.6%.

***N*-Benzyl-2-chloroacetamide**



At 0 °C under N_2, chloroacetyl chloride (7.65 mL, 96.1 mmol, 1.05 eq.) was added slowly to solution of benzylamine (10.0 mL, 91.6 mmol, 1.00 eq.) and pyridine (14.7 mL, 183 mmol, 2.00 eq.) in THF (350 mL). The reaction mixture was stirred for 5 h while slowly warming up to room temperature. Water was added and the aqueous layer was extracted with EtOAc (3 x 200 mL). The combined organic layers were washed with water, brine, dried (Na_2SO_4) and concentrated *in vacuo*.

Colorless solid, R_f = 0.10 (cHex/EtOAc 90:10), yield 14.4 g (86%).

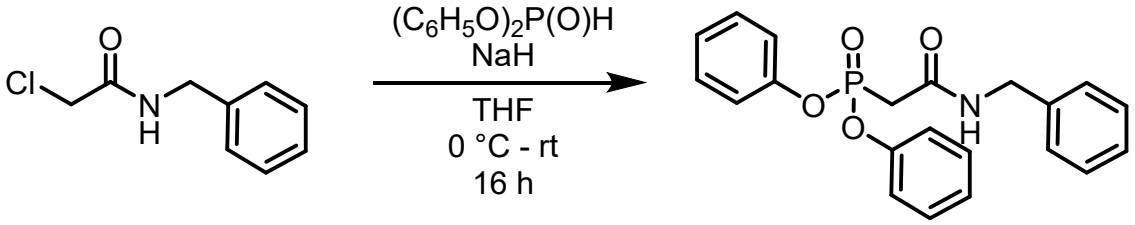
$C_9H_{10}ClNO$ (183.6 g/mol).

Analytical data in accordance with literature.[7]

HRMS: m/z = 184.0510, calcd. 184.0524 for $C_9H_{11}ClNO^+$ $[M+H]^+$.

Purity (HPLC): 95.5% (t_R = 14.0 min).

Diphenyl 1 [(benzylamino)carbonyl]methanephosphonate



Synthesis procedure was adapted from Kojima et al.[8]

At 0 °C under N_2, NaH (60% dispersion in mineral oil, 7,07 g, 177 mmol, 3.00 eq.) was suspended in THF (120 mL). Diphenylphosphite (34.0 mL, 177 mmol, 3.00 eq.) was added dropwise and the solution was stirred for 1 h at 0 °C. *N*-Benzyl-2-chloroacetamide (10.0 g, 59.0 mmol, 1.00 eq.) dissolved in THF (10 mL) was added dropwise to the reaction mixture and the mixture was stirred for 16 h while slowly warming up to room temperature. Aqueous NH_4Cl solution (1/2 conc., 100 mL) was added and the precipitate was filtered off. The solid was washed with water (3 x 50 mL) and cHex (3 x 50 mL) and dried *in vacuo*. The product was used without further purification.

Colorless solid, mp 145 – 147 °C, R_f = 0.25 (cHex/EtOAc 75:25), yield 16.9 g (78%).

$C_{21}H_{20}NO_4P$ (381.4 g/mol).

Analytical data in accordance with literature.[8]

HRMS: m/z = 382.1211, calcd. 382.1203 for $C_{21}H_{21}NO_4P$ $[M+H]^+$.

Purity (HPLC): 91.7% (t_R = 18.9 min).

X-ray crystal structure analysis of 8b (dan10126)

A colorless plate-like specimen of $C_{25}H_{29}NO_3$, approximate dimensions 0.030 mm x 0.120 mm x 0.200 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Kappa CCD Bruker APEXII Diffractometer system equipped with a fine-focus sealed tube Cu sealed tube (CuKα, λ = 1.54178 Å) and a graphite monochromator. A total of 1740 frames were collected. The total exposure time was 22.74 hours. The frames were integrated with the Bruker SAINT software package using a wide-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 38113 reflections to a maximum θ angle of 66.90° (0.84 Å resolution), of which 4226 were independent (average redundancy 9.019, completeness = 99.8%, R_{int} = 13.27%, R_{sig} = 7.31%) and 3057 (72.34%) were greater than $2\sigma(F^2)$. The final cell constants of a = 27.6191(12) Å, b = 9.9208(5) Å, c = 20.1969(8) Å, β = 120.649(2)°, volume = 4761.0(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 4740 reflections above 20 σ(I) with 7.441° < 2θ < 132.7°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.857. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.8960 and 0.9830. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group *C*2/*c*, with Z = 8 for the formula unit, $C_{25}H_{29}NO_3$. The final anisotropic full-matrix least-squares refinement on F^2 with 263 variables converged at R1 = 5.00%, for the observed data and wR2 = 12.57% for all data. The goodness-of-fit was 1.033. The largest peak in the final difference electron density synthesis was 0.244 $e^-/Å^3$ and the largest hole was -0.272 $e^-/Å^3$ with an RMS deviation of 0.052 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.092 g/cm^3 and F(000), 1680 e^-. CCDC Nr.: 2279510.

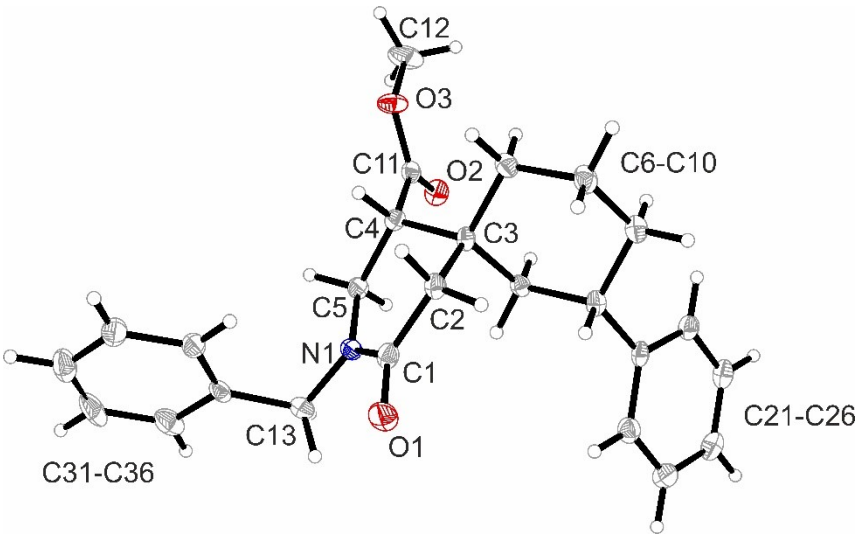


Figure S1: Crystal structure of compound **8b**. Thermal ellipsoids are set at 50% probability.

Table 1. Sample and crystal data for dan10126.

Identification code	dan10126	
Chemical formula	$C_{25}H_{29}NO_3$	
Formula weight	391.49 g/mol	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal size	0.030 x 0.120 x 0.200 mm	
Crystal habit	colorless plate	
Crystal system	monoclinic	
Space group	C 1 2/c 1	
Unit cell dimensions	a = 27.6191(12) Å	α = 90°
	b = 9.9208(5) Å	β = 120.649(2)°
	c = 20.1969(8) Å	γ = 90°
Volume	4761.0(4) $Å^3$	
Z	8	
Density (calculated)	1.092 g/cm^3	
Absorption coefficient	0.563 mm^{-1}	
F(000)	1680	

Table 2. Data collection and structure refinement for dan10126.

Diffractometer	Kappa CCD Bruker APEXII Diffractometer	
Radiation source	fine-focus sealed tube Cu sealed tube (CuKα, λ = 1.54178 Å)	
Theta range for data collection	3.72 to 66.90°	
Index ranges	-32<=h<=32, -11<=k<=11, -24<=l<=24	
Reflections collected	38113	
Independent reflections	4226 [R(int) = 0.1327]	
Coverage of independent reflections	99.8%	
Absorption correction	Multi-Scan	
Max. and min. transmission	0.9830 and 0.8960	
Structure solution technique	direct methods	
Structure solution program	SHELXT 2018/2 (Sheldrick, 2018)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	4226 / 0 / 263	
Goodness-of-fit on F^2	1.033	
Final R indices	3057 data; I>2σ(I)	R1 = 0.0500, wR2 = 0.1130
	all data	R1 = 0.0750, wR2 = 0.1257
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0335P)^2+4.6723P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.244 and -0.272 $eÅ^{-3}$	
R.M.S. deviation from mean	0.052 $eÅ^{-3}$	

Table 3. Bond lengths (Å) for dan10126.

N1-C1	1.351(3)	N1-C13	1.458(3)
N1-C5	1.460(3)	O1-C1	1.239(2)
O2-C11	1.209(2)	O3-C11	1.340(2)
O3-C12	1.455(3)	C1-C2	1.509(3)
C2-C3	1.541(3)	C2-H2A	0.99
C2-H2B	0.99	C3-C10	1.536(3)
C3-C6	1.543(3)	C3-C4	1.551(3)
C4-C11	1.516(3)	C4-C5	1.520(3)
C4-H4	1.0	C5-H5A	0.99
C5-H5B	0.99	C6-C7	1.544(3)
C6-H6A	0.99	C6-H6B	0.99
C7-C21	1.516(3)	C7-C8	1.526(3)
C7-H7	1.0	C8-C9	1.531(3)
C8-H8A	0.99	C8-H8B	0.99
C9-C10	1.532(3)	C9-H9A	0.99
C9-H9B	0.99	C10-H10A	0.99
C10-H10B	0.99	C12-H12A	0.98
C12-H12B	0.98	C12-H12C	0.98
C13-C31	1.518(3)	C13-H13A	0.99
C13-H13B	0.99	C21-C26	1.392(3)
C21-C22	1.394(3)	C22-C23	1.386(3)
C22-H22	0.95	C23-C24	1.386(3)
C23-H23	0.95	C24-C25	1.380(3)
C24-H24	0.95	C25-C26	1.390(3)
C25-H25	0.95	C26-H26	0.95
C31-C32	1.388(3)	C31-C36	1.398(3)
C32-C33	1.392(3)	C32-H32	0.95
C33-C34	1.373(4)	C33-H33	0.95
C34-C35	1.375(4)	C34-H34	0.95
C35-C36	1.403(4)	C35-H35	0.95
C36-H36	0.95		

Table 4. Bond angles (°) for dan10126.

C1-N1-C13	120.17(17)	C1-N1-C5	125.17(17)
C13-N1-C5	114.66(16)	C11-O3-C12	115.93(18)
O1-C1-N1	121.96(19)	O1-C1-C2	120.40(19)
N1-C1-C2	117.61(17)	C1-C2-C3	114.83(16)
C1-C2-H2A	108.6	C3-C2-H2A	108.6
C1-C2-H2B	108.6	C3-C2-H2B	108.6
H2A-C2-H2B	107.5	C10-C3-C2	110.57(16)
C10-C3-C6	109.11(16)	C2-C3-C6	110.50(16)
C10-C3-C4	110.68(16)	C2-C3-C4	103.54(15)
C6-C3-C4	112.36(16)	C11-C4-C5	108.24(16)

C11-C4-C3	113.13(16)	C5-C4-C3	111.53(16)
C11-C4-H4	107.9	C5-C4-H4	107.9
C3-C4-H4	107.9	N1-C5-C4	113.66(16)
N1-C5-H5A	108.8	C4-C5-H5A	108.8
N1-C5-H5B	108.8	C4-C5-H5B	108.8
H5A-C5-H5B	107.7	C3-C6-C7	112.65(16)
C3-C6-H6A	109.1	C7-C6-H6A	109.1
C3-C6-H6B	109.1	C7-C6-H6B	109.1
H6A-C6-H6B	107.8	C21-C7-C8	115.28(17)
C21-C7-C6	109.69(16)	C8-C7-C6	110.19(16)
C21-C7-H7	107.1	C8-C7-H7	107.1
C6-C7-H7	107.1	C7-C8-C9	110.27(17)
C7-C8-H8A	109.6	C9-C8-H8A	109.6
C7-C8-H8B	109.6	C9-C8-H8B	109.6
H8A-C8-H8B	108.1	C8-C9-C10	111.29(17)
C8-C9-H9A	109.4	C10-C9-H9A	109.4
C8-C9-H9B	109.4	C10-C9-H9B	109.4
H9A-C9-H9B	108.0	C9-C10-C3	113.33(17)
C9-C10-H10A	108.9	C3-C10-H10A	108.9
C9-C10-H10B	108.9	C3-C10-H10B	108.9
H10A-C10-H10B	107.7	O2-C11-O3	124.01(19)
O2-C11-C4	125.05(18)	O3-C11-C4	110.94(17)
O3-C12-H12A	109.5	O3-C12-H12B	109.5
H12A-C12-H12B	109.5	O3-C12-H12C	109.5
H12A-C12-H12C	109.5	H12B-C12-H12C	109.5
N1-C13-C31	112.45(16)	N1-C13-H13A	109.1
C31-C13-H13A	109.1	N1-C13-H13B	109.1
C31-C13-H13B	109.1	H13A-C13-H13B	107.8
C26-C21-C22	118.29(18)	C26-C21-C7	123.05(19)
C22-C21-C7	118.65(18)	C23-C22-C21	121.36(19)
C23-C22-H22	119.3	C21-C22-H22	119.3
C24-C23-C22	119.7(2)	C24-C23-H23	120.2
C22-C23-H23	120.2	C25-C24-C23	119.6(2)
C25-C24-H24	120.2	C23-C24-H24	120.2
C24-C25-C26	120.7(2)	C24-C25-H25	119.6
C26-C25-H25	119.6	C25-C26-C21	120.3(2)
C25-C26-H26	119.8	C21-C26-H26	119.8
C32-C31-C36	118.3(2)	C32-C31-C13	122.00(18)
C36-C31-C13	119.7(2)	C31-C32-C33	121.0(2)
C31-C32-H32	119.5	C33-C32-H32	119.5
C34-C33-C32	120.3(2)	C34-C33-H33	119.8
C32-C33-H33	119.8	C33-C34-C35	119.9(2)
C33-C34-H34	120.0	C35-C34-H34	120.0
C34-C35-C36	120.3(2)	C34-C35-H35	119.9
C36-C35-H35	119.9	C31-C36-C35	120.2(2)

C31-C36-H36	119.9	C35-C36-H36	119.9

Table 5. Torsion angles (°) for dan10126.

C13-N1-C1-O1	3.7(3)	C5-N1-C1-O1	-175.87(19)
C13-N1-C1-C2	-174.13(17)	C5-N1-C1-C2	6.3(3)
O1-C1-C2-C3	152.38(19)	N1-C1-C2-C3	-29.7(3)
C1-C2-C3-C10	174.56(17)	C1-C2-C3-C6	-64.5(2)
C1-C2-C3-C4	56.0(2)	C10-C3-C4-C11	56.5(2)
C2-C3-C4-C11	175.02(16)	C6-C3-C4-C11	-65.7(2)
C10-C3-C4-C5	178.82(16)	C2-C3-C4-C5	-62.67(19)
C6-C3-C4-C5	56.6(2)	C1-N1-C5-C4	-13.5(3)
C13-N1-C5-C4	166.90(16)	C11-C4-C5-N1	168.46(16)
C3-C4-C5-N1	43.4(2)	C10-C3-C6-C7	54.0(2)
C2-C3-C6-C7	-67.8(2)	C4-C3-C6-C7	177.12(15)
C3-C6-C7-C21	174.46(16)	C3-C6-C7-C8	-57.6(2)
C21-C7-C8-C9	-177.63(17)	C6-C7-C8-C9	57.6(2)
C7-C8-C9-C10	-56.6(2)	C8-C9-C10-C3	55.2(2)
C2-C3-C10-C9	69.0(2)	C6-C3-C10-C9	-52.8(2)
C4-C3-C10-C9	-176.89(16)	C12-O3-C11-O2	0.3(3)
C12-O3-C11-C4	179.63(18)	C5-C4-C11-O2	-46.5(3)
C3-C4-C11-O2	77.6(3)	C5-C4-C11-O3	134.24(17)
C3-C4-C11-O3	-101.63(19)	C1-N1-C13-C31	98.4(2)
C5-N1-C13-C31	-82.0(2)	C8-C7-C21-C26	-31.8(3)
C6-C7-C21-C26	93.2(2)	C8-C7-C21-C22	149.38(19)
C6-C7-C21-C22	-85.6(2)	C26-C21-C22-C23	-0.1(3)
C7-C21-C22-C23	178.7(2)	C21-C22-C23-C24	0.3(3)
C22-C23-C24-C25	-0.3(3)	C23-C24-C25-C26	0.1(3)
C24-C25-C26-C21	0.1(3)	C22-C21-C26-C25	-0.1(3)
C7-C21-C26-C25	-178.90(19)	N1-C13-C31-C32	-27.3(3)
N1-C13-C31-C36	154.79(19)	C36-C31-C32-C33	0.4(3)
C13-C31-C32-C33	-177.54(19)	C31-C32-C33-C34	-0.3(3)
C32-C33-C34-C35	-0.1(4)	C33-C34-C35-C36	0.4(4)
C32-C31-C36-C35	-0.2(3)	C13-C31-C36-C35	177.8(2)
C34-C35-C36-C31	-0.2(3)		

Receptor binding studies

Materials

Guinea pig brains, rat brains and rat livers were commercially available (Harlan-Winkelmann, Borchen, Germany). The recombinant L(tk-) cells stably expressing the GluN2B receptor were obtained from Prof. Dr. Dieter Steinhilber (Frankfurt, Germany). Homogenizers: Elvehjem Potter (B. Braun Biotech International, Melsungen, Germany) and Soniprep® 150 (MSE, London, UK). Centrifuges: Cooling centrifuge model Eppendorf 5427R (Eppendorf, Hamburg, Germany) and High-speed cooling centrifuge model Sorvall® RC-5C plus (Thermo Fisher Scientific, Langenselbold, Germany). Multiplates: standard 96 well multiplates (Diagonal, Muenster, Germany). Shaker: self-made device with adjustable temperature and tumbling speed (scientific workshop of the institute). Harvester: MicroBeta® FilterMate 96 Harvester. Filter: Printed Filtermat Typ A and B. Scintillator: Meltilex® (Typ A or B) solid state scintillator. Scintillation analyzer: MicroBeta® Trilux (all Perkin Elmer LAS, Rodgau-Jügesheim, Germany).

Preparation of membrane homogenates from guinea pig brain

5 guinea pig brains were homogenized with the potter (500-800 rpm, 10 up and down strokes) in 6 volumes of cold 0.32 M sucrose. The suspension was centrifuged at 1,200 x g for 10 min at 4 °C. The supernatant was separated and centrifuged at 23,500 x g for 20 min at 4 °C. The pellet was resuspended in 5-6 volumes of buffer (50 mM TRIS, pH 7.4) and centrifuged again at 23,500 x g (20 min, 4 °C). This procedure was repeated twice. The final pellet was resuspended in 5-6 volumes of buffer and frozen (-80 °C) in 1.5 mL portions containing about 1.5 mg protein/mL.

Preparation of membrane homogenates from rat brain

5 rat brains (species: Sprague Dawley rats) were homogenized with the potter (500-800 rpm, 10 up and down strokes) in 6 volumes of cold 0.32 M sucrose. The suspension was centrifuged at 1,200 x g for 10 min at 4 °C. The supernatant was separated and centrifuged at 23,500 x g for 20 min at 4 °C. The pellet was resuspended in 5-6 volumes of buffer (50 mM TRIS, pH 7.4) and centrifuged again at 23,500 x g (20 min, 4 °C). This procedure was repeated twice. The final pellet was resuspended in 5-6 volumes of buffer and frozen (-80 °C) in 1.5 mL portions containing about 1.5 mg protein/mL.

Preparation of membrane homogenates from rat liver

Two rat livers were cut into small pieces and homogenized with the potter (500-800 rpm, 10 up and down strokes) in 6 volumes of cold 0.32 M sucrose. The suspension was centrifuged at 1,200 x g for 10 min at 4 °C. The supernatant was separated and centrifuged at 31,000 x g for 20 min at 4 °C. The pellet was resuspended in 5-6 volumes of buffer (50 mM TRIS, pH 8.0) and incubated at rt for 30 min. After the incubation, the suspension was centrifuged again at 31,000 x g for 20 min at 4 °C. The final pellet was resuspended in 5-6 volumes of buffer and stored at -80 °C in 1.5 mL portions containing about 2 mg protein/mL.

Cell culture and preparation of membrane homogenates from GluN2B cells

Mouse L(tk-) cells stably transfected with the dexamethasone-inducible eukaryotic expression vectors pMSG GluN1a, pMSG GluN2B (1:5 ratio) were grown in Modified Earl's Medium (MEM) containing 10 % of standardized FBS Superior (Biochrom AG, Berlin, Germany). The expression of the NMDA receptor at the cell surface was induced after the cell density of the adherent growing cells had reached approximately 90 % of confluency. For the induction, the original growth medium was replaced by growth medium containing 4 µM dexamethasone and 4 µM ketamine (final concentration). After 24 h, the cells were rinsed with phosphate buffered saline solution (PBS, Biochrom AG, Berlin, Germany), harvested by mechanical detachment and pelleted (10 min, 1,200 x g).

For the binding assay, the cell pellet was resuspended in PBS solution and the number of cells was determined using a Scepter® cell counter (MERCK Millipore, Darmstadt, Germany). Subsequently, the cells were lysed by sonication (4 °C, 6 x 10 s cycles with breaks of 10 s). The resulting cell fragments were centrifuged with a high performance cool centrifuge (23,500 x g, 4 °C). The supernatant was discarded and the pellet was resuspended in a defined volume of PBS yielding cell fragments of approximately 500,000 cells/mL. The suspension of membrane homogenates was sonicated again (4 °C, 2 x 10 s cycles with a break of 10 s) and stored at -80 °C.

Protein determination

The protein concentration was determined by the method of Bradford,[9] modified by Stoscheck.[10] The Bradford solution was prepared by dissolving 5 mg of Coomassie Brilliant Blue G 250 in 2.5 mL of EtOH (95 %, v/v). 10 mL deionized H_2O and 5 mL phosphoric acid (85 %, m/v) were added to this solution, the mixture was stirred and filled to a total volume of 50 mL with deionized water. The calibration was carried out using bovine serum albumin

as a standard in 9 concentrations (0.1, 0.2, 0.4, 0.6, 0.8, 1.0, 1.5, 2.0 and 4.0 mg /mL). In a 96 well standard multiplate, 10 µL of the calibration solution or 10 µL of the membrane receptor preparation were mixed with 190 µL of the Bradford solution, respectively. After 5 min, the UV absorption of the protein-dye complex at λ = 595 nm was measured with a plate reader (Tecan Genios®, Tecan, Crailsheim, Germany).

General procedures for the binding assays

The test compound solutions were prepared by dissolving approximately 10 µmol (usually 2-4 mg) of test compound in DMSO so that a 10 mM stock solution was obtained. To obtain the required test solutions for the assay, the DMSO stock solution was diluted with the respective assay buffer. The filtermats were presoaked in 0.5 % aqueous polyethylenimine solution for 2 h at rt before use. All binding experiments were carried out in duplicates in the 96 well multiplates. The concentrations given are the final concentration in the assay. Generally, the assays were performed by addition of 50 µL of the respective assay buffer, 50 µL of test compound solution in various concentrations (10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}, 10^{-9} and 10^{-10} mol/L), 50 µL of the corresponding radioligand solution and 50 µL of the respective receptor preparation into each well of the multiplate (total volume 200 µL). The receptor preparation was always added last. During the incubation, the multiplates were shaken at a speed of 500-600 rpm at the specified temperature. Unless otherwise noted, the assays were terminated after 120 min by rapid filtration using the harvester. During the filtration, each well was washed five times with 300 µL of water. Subsequently, the filtermats were dried at 95 °C. The solid scintillator was melted on the dried filtermats at a temperature of 95 °C for 5 min. After solidifying of the scintillator at rt, the trapped radioactivity in the filtermats was measured with the scintillation analyzer. Each position on the filtermat corresponding to one well of the multiplate was measured for 5 min with the [^{3}H]-counting protocol. The overall counting efficiency was 20 %. The IC_{50} values were calculated with the program GraphPad Prism® 3.0 (GraphPad Software, San Diego, CA, USA) by non-linear regression analysis. Subsequently, the IC_{50} values were transformed into K_i values using the equation of Cheng and Prusoff.[11] The K_i values are given as mean value ± SEM from three independent experiments. For test compounds showing low affinity (K_i > 100 nM), only a single experiment was performed.

Performance of the binding assays

σ_2 receptor assay

The assays were performed with the radioligand [^{3}H]di-*o*-tolylguanidine (specific activity 50 Ci/mmol; ARC, St. Louis, MO, USA). The thawed rat liver membrane preparation (about 100 µg protein) was incubated with various concentrations of the test compound, 3 nM [^{3}H]di-*o*-tolylguanidine and buffer containing (+)-pentazocine (500 nM (+)-pentazocine in TRIS buffer (50 mM TRIS, pH 8.0)) at rt. The non-specific binding was determined with 10 µM non-labeled di-*o*-tolylguanidine. The K_d value of di-*o*-tolylguanidine is 17.9 nM.[12]

Ifenprodil binding site of GluN2B subunit containing NMDA receptors

The competitive binding assay was performed with the radioligand [^{3}H]ifenprodil (60 Ci/mmol; BIOTREND, Cologne, Germany). The thawed cell membrane preparation from the transfected L(tk-) cells (about 20 µg protein) was incubated with various concentrations of test compounds, 5 nM [^{3}H]ifenprodil, and TRIS/EDTA-buffer (5 mM TRIS/1 mM EDTA, pH 7.5) at 37 °C. The non-specific binding was determined with 10 µM unlabeled ifenprodil. The K_d value of ifenprodil is 7.6 nM.[13]

KOR assay

The assay was performed with the radioligand [^{3}H]U-69,593 (55 Ci/mmol, BIOTREND). The thawed guinea pig brain membrane preparation (about 100 µg of the protein) was incubated with various concentrations of test compounds, 1 nM [^{3}H]U-69,593, and TRIS-$MgCl_2$-buffer (50 mM TRIS, 8 mM $MgCl_2$, pH 7.4) at 37 °C. The non-specific binding was determined with 10 µM unlabeled U-69,593. The K_d value of U-69,593 is 0.69 nM.

MOR assay

The assay was performed with the radioligand [^{3}H]DAMGO (51 Ci/mmol, Perkin Elmer). The thawed guinea pig brain membrane preparation (about 100 µg of the protein) was incubated with various concentrations of test compounds, 3 nM [^{3}H]DAMGO, and TRIS-$MgCl_2$-buffer (50 mM TRIS, 8 mM $MgCl_2$, pH 7.4) at 37 °C. The non-specific binding was determined with 10 µM unlabeled naloxone. The K_d value of DAMGO is 0.57 nM.

DOR assay

The assay was performed with the radioligand [^{3}H]DPDPE (69 Ci/mmol, BIOTREND). The thawed rat brain membrane preparation (about 75 µg of the protein) was incubated with various concentrations of test compounds, 3 nM [^{3}H]DPDPE, and TRIS-$MgCl_2$-buffer (50 mM TRIS, 8 mM $MgCl_2$, pH 7.4) supplemented with SIGMAFAST® protease inhibitor mix (Sigma Aldrich Biochemicals, Hamburg, Germany; 1 tablet dissolved in 100 mL of buffer) at 37 °C. The non-specific binding was determined with 10 µM unlabeled morphine. The K_d value of DPDPE is 0.65 nM.

Quantum chemical Calculations

All calculations were performed using the GAUSSIAN 16, B.01 package of programs.[14] The structures were fully optimized first using the B3LYP/6-31G(d)[15,16] +GD3BJ[17,18] method, then the TPSSTPSS/def2tzvp[19] + GD3BJ, then the PBE1PBE/def2tzvp[20–24] +GD3BJ methods and finally the wB97X-D/def2tzvp functional[25] all including the PCM-solvent sphere for dichloroethane.[26] Zeropoint vibrational energies and free enthalpy contributions were determined analytically.

Table 6: Total energies (E_{tot}) and Gibbs free energies (G_{298}) [a.u.], of the cycloadducts, respectively, the respective transition states and the relative energies with respect to the sum of the two educts **G** and methylacrylate (last column) [kcal/mol].

Species	E_{tot} [a.u.]	E_{rel} [kcal/mol]	G_{298} [a.u.]	E_{rel} [kcal/mol]
B3LYP				
1-Azabutadiene G	-890,77207		-890,49023	
Methylacrylate	-306,49495		-306,43000	
Sum	-1197,26702	0.00	-1196,92023	0.00
vdW-Complex	-1197,27933	-7,72	-1196,91210	5,10
TS_Diels-Alder	-1197,25047	10,39	-1196,87774	26,66
Min H	-1197,31187	-28,14	-1196,93240	-7,64
TPSSTPSS				
1-Azabutadiene G	-891,07243		-890,79747	
Methylacrylate	-306,65378		-306,59087	
Sum	-1197,72621	0,00	-1197,38834	0,00
vdW-Complex	-1197,73283	-4,16	-1197,37728	6,94
TS-Diels-Alder	-1197,70974	10,33	-1197,34634	26,35
Min-H	-1197,76003	-21,22	-1197,39077	-1,52
PBE1PBE				
1-Azabutadiene G	-890,09425		-889,81289	
Methylacrylate	-306,25109		-306,18608	
Sum	-1.196,34534	0,00	-1.195,99897	0,00
vdW-Complex	-1.196,35286	-4,72	-1.195,98836	6,66
TS-C..N	-1.196,32884	10,36	-1.196,32884	25,88
Dipolar Interm.	-1.196,34153	2,39	-1.195,96832	19,23
TS-C..C	-1.196,33480	6,61	-1.195,96110	23,76
Min-H	-1.196,39806	-33,08	-1.196,01899	-12,56

wB97X-D				
1-Azabutadiene G	-890,72202		-890,43765	
Methylacrylate	-306,49442		-306,42899	
Sum	-1.197,21644	0,00	-1.196,86664	0,00
vdW-Complex	-1.197,22267	-3,91	-1.196,85295	8,59
TS-C..N	-1.197,19509	13,14	-1.196,82024	29,12
Dipolar-Interm	-1.197,20674	6,09	-1.196,83114	22,28
TS-C..C	-1.197,19628	12.65	-1.196,81951	29,57
Min-H	-1.197,26300	-29,22	-1.196,88153	-9,34

Gaussian Archive Entries

(Total energies (a.u.), number of imaginary frequencies (for transition states: imaginary frequencies), coordinates)

B3LYP
2-Silyloxy-1-azabutadiene G
HF=-890.772072 a.u. (0)
1\1\GINC-R03N37\FOpt\RB3LYP\6-31G(d,p)\C12H23N1O1Si1\WURTHWE\27-Apr-2023\0\\#
b3lyp/6-31G(d,p) opt=readfc geom=check guess=read freq pop=nbo emp=gd3bj
scrf=(solvent=dichloroethane)\\ 2-Silyloxy-1-azabutadiene G \\0,1\
C,-0.35345846,-0.0776504467,-0.0972121299\C,-0.1447082285,0.0826411484,1.3861496218\
C,1.2913696466,0.3382276772,1.7698981928\C,2.1 935686583,-0.7953344801,1.2374128303\
C,2.00936621,-0.9924206544,-0.272641556\C,0.5356655108,-1.2180628473,-0.6338610988\
C,-1.1008743936,-0.0354039187,2.323856141\C,-2.531688712,-0.3170043677,2.1001001404\
O,-3.3898562216,0.3917357332,2.9012447422\N,-2.9514603609,-1.1921532534,1.2722964553\
C,-4.3961061371,-1.3434306882,1.1340527506\H,1.3946240128,0.4376766707,2.8550390423\
H,1.6207346959,1.2859519939,1.3197084612\H,1.9352796216,-1.7251710424,1.7603510858\
H,3.2408924161,-0.5758391894,1.472589327\H,2.6187866317,-1.8346318346,-0.6196408934\
H,2.3753699845,-0.1000209018,-0.7992170984\H,0.1891470366,-2.1643014053,-0.1991982353\
H,0.4150071262,-1.300806495,-1.7196729192\H,-1.4014542898,-0.2664053259,-0.3265562192\
H,-0.0508096813,0.8582717939,-0.5901333703\H,-0.8323129553,0.1309057389,3.3649586004\
Si,-3.3907651473,2.0846732236,3.1208556017\H,-4.6060112685,-2.047967444,0.3252916482\
H,-4.8956552517,-0.3924819027,0.9080876886\H,-4.8525319767,-1.7311022766,2.0537391165\
C,-5.1087437088,2.4428806392,3.7744898599\C,-2.0876399592,2.601518729,4.3701956973\
C,-3.0853026071,2.8851627928,1.451486051\H,-3.1238428756,3.9767120463,1.5326909176\
H,-2.1009050582,2.6098735951,1.0606205997\H,-3.8401615788,2.5728039071,0.7226674416\
H,-5.2349505613,3.51498823,3.9593576427\H,-5.8754875589,2.1290791028,3.0594489839\
H,-5.2875866579,1.9164169188,4.7175440301\H,-2.2203382366,3.6577926711,4.6302167466\
H,-2.1711492253,2.0172439912,5.2923858289\H,-1.075181278,2.4765138505,3.9766659879
\\Version=ES64L-G16RevB.01\State=1-A\HF=-890.772072\RMSD=3.590e-09\RMSF=9.584e-
07\Dipole=0.4004485,1.2152371,0.2081827\Quadrupole=2.7699243,-2.2723725,-0.4975518,-
2.7239098,-0.8458587,0.8952872\PG=C01 [X(C12H23N1O1Si1)]\\@

Methyl acrylate
HF=-306.4949522 a.u. (0)
1\1\GINC-R02N47\FOpt\RB3LYP\6-31G(d,p)\C4H6O2\WURTHWE\21-Jun-2023\0\\# b3lyp/6-
31G(d,p) Opt emp=gd3bj Pop=NBO Freq scrf=(solvent=dichloroethane)\\methyl acrylate)\\0,1\
C,0.0196121855,0.,0.0136187591\O,0.0222798579,0.,1.2322464022\
C,1.219862861,0.,-0.8559471521\C,2.4452411674,0.,-0.3277052889\
O,-1.1075038187,0.,-0.7281250474\C,-2.3390321404,0.,0.0156991164\
H,1.050161181,0.,-1.9274724541\H,2.5798469904,0.,0.7494919818\
H,3.3333648508,0.,-0.9500935663\H,-3.1328885273,0.,-0.7293823096\
H,-2.4046346693,-0.8898233073,0.6456113863\H,-2.4046346693,0.8898233073,0.6456113863\\
Version=ES64L-G16RevB.01\State=1-A'\HF=-306.4949522\RMSD=4.427e-09\RMSF=6.082e-
05\Dipole=-0.1003371,0.,-0.7231601\Quadrupole=6.0688336,-2.0498695,-4.0189642,0.,-
1.5104814,0.\PG=CS [SG(C4H4O2),X(H2)]\\@

Van der Waals Complex
HF=-1197.2793286 a.u. (0)
1\1\GINC-R02N31\FOpt\RB3LYP\6-31G(d,p)\C16H29N1O3Si1\WURTHWE\27-Apr-2023\0\\#
b3lyp/6-31G(d,p) opt=readfc geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\Van der Waals Complex\\0,1\

C,-0.3598564188,0.1849346213,-0.185889427\C,-0.3481110073,0.2095948813,1.3471273238\
C,1.0584727971,-0.0606317715,1.8937826395\C,2.0872218777,0.9217689217,1.3005406127\
C,2.0344110334,0.9172368728,-0.2077607735\C,0.6629341713,1.1787102336,-0.7724189905\
C,3.1539362657,0.679234036,-0.9164617191\C,3.3280732006,0.6569321392,-2.3784471112\
N,2.3863660216,0.3996693806,-3.2028217057\C,2.7055588549,0.4591289302,-4.6223062951\
O,4.5839433028,0.9492815648,-2.8325445396\Si,6.1199375461,1.0894739614,-2.1112500331\
C,6.5329739463,-0.481402711,-1.1656913624\C,7.2583918845,1.2730555248,-3.5872759787\
C,6.2078613651,2.6120545236,-1.0167901737\C,1.9014143672,3.9428830987,-2.8326414405\
C,2.7916698502,3.9124290862,-1.838804331\C,2.4807712797,4.22689618,-0.4286665933\
O,1.2062267482,4.6328921453,-0.2435992991\C,0.8401365368,4.9533717753,1.1095612132\
O,3.2858309123,4.1308742014,0.4836604722\H,3.8194551984,3.6175955173,-2.0084237741\
H,0.8671599645,4.2188965374,-2.6607422989\H,2.1880355648,3.6787186963,-3.8447898475\
H,4.0674368874,0.5327271091,-0.3488912526\H,3.0963265402,0.68750781,1.6539123086\
H,1.8538931313,1.935279581,1.6554743139\H,0.6827224406,1.12761465,-1.8592255417\
H,0.3642918978,2.1946277441,-0.4785302478\H,-1.3595918364,0.4221062594,-0.5664548957\
H,-0.1164651369,-0.8261686381,-0.5375420342\H,-1.0567052557,-0.5250475638,1.7464746318\
H,-0.6861859585,1.1964901122,1.6933977013\H,1.3573395304,-1.0850231264,1.6357496948\
H,1.0691375772,0.0092823953,2.9871603452\H,6.343874126,-1.3650937052,-1.7838158863\
H,5.9660003176,-0.5903910456,-0.2370990497\H,7.5973401114,-0.4779832049,-0.9049839312\
H,7.2233193422,0.3855564647,-4.2267896324\H,8.2937711834,1.4125155711,-3.2582313624\
H,6.9783315799,2.1404463057,-4.1933496629\H,5.3807650091,2.6829496795,-0.3052723446\
H,6.2004914926,3.5229022574,-1.6250449721\H,7.1463200619,2.6038667649,-0.4507294799\
H,1.8159616588,0.1979790368,-5.2013155276\H,3.0342256599,1.4618463355,-4.9276281753\
H,3.5135975547,-0.232146842,-4.8955711394\H,-0.1715192152,5.3517962019,1.0523067136\
H,0.8574661624,4.0567756101,1.7335278108\H,1.5237429156,5.6950902109,1.5266617776
\\Version=ES64L-G16RevB.01\State=1-A\HF=-1197.2793286\RMSD=4.961e-09\RMSF=6.496e-
06\Dipole=0.0889427,0.4396522,0.366197\Quadrupole=4.9938586,-3.849892,-1.1439666,-
7.29847,-6.1634322,-2.5222166\PG=C01 [X(C16H29N1O3Si1)]\\@

TS-Diels-Alder

HF=-1197.250468 a.u. (1, -207.8175 cm^{-1})
1\1\GINC-R01N40\FTS\RB3LYP\6-31G(d,p)\C16H29N1O3Si1\WURTHWE\27-Apr-2023\0\\#
b3lyp/6-31G(d,p) Opt=(ts,noeigentest,readfc) geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\TS-Diels-Alder\\0,1\
C,0.1582692492,-0.2089956442,0.9860296644\C,0.6000170578,0.194332683,2.395978923\
C,2.1329002585,0.3186360436,2.4884295488\C,2.8445294437,-0.8925297444,1.9522026271\
C,2.3960187683,-1.3441323522,0.5855463556\C,0.8607405997,-1.497479169,0.5493932917\
C,3.6887307828,-1.596709715,2.7490874934\C,4.5803272301,-2.6264225667,2.2915555672\
O,4.852766217,-3.6709919738,3.0876483875\Si,3.7474257995,-4.4905705078,4.1360308813\
C,4.6341214573,-6.1035045787,4.4620230088\N,5.2033689213,-2.5561145175,1.1381198588\
C,5.995036647,-3.7068281305,0.7048436201\C,3.5135710228,-3.5096596383,5.7152014125\
C,2.1430419653,-4.7272284587,3.1989658968\C,5.8382220003,-1.1355243026,0.4847184622\
C,5.3814282919,0.1387397828,0.948307971\C,4.622502859,1.0508557332,0.1910898151\
O,4.2057251352,2.1644857791,0.5565115672\O,4.3398058846,0.6112829569,-1.1074137024\
C,3.5668279029,1.5140124984,-1.8930165412\H,5.6498919096,0.4764930735,1.9421286696\
H,5.664266155,-1.3037101676,-0.5757289121\H,6.8754588894,-1.366560159,0.7439294204\
H,3.7882028569,-1.3232706577,3.7958243104\H,2.4448640687,0.5187485909,3.5181671008\
H,2.4692883294,1.1701541998,1.8784032752\H,2.8817625505,-2.2798680595,0.3061348392\
H,2.6928123799,-0.6019846601,-0.1599085248\H,0.5572648638,-1.7815104693,-0.4640615084\
H,0.5588189246,-2.3192984023,1.2125030032\H,-0.9295970979,-0.3360855582,0.9509415885\
H,0.4083979473,0.5958724744,0.2812793094\H,0.258468295,-0.5647274455,3.1121790889\
H,0.1391142331,1.1424405806,2.6927573181\H,2.3160771745,-5.2426506239,2.2488504738\
H,1.6640208809,-3.7679024524,2.9862532524\H,1.4474119171,-5.3326659831,3.789643956\
H,4.8045580681,-6.6542232374,3.5319107497\H,4.0399199648,-6.7377895241,5.1281120407\
H,5.6038517448,-5.9298398583,4.9388913553\H,2.904205882,-2.6155468506,5.5585241954\

H,4.476935996,-3.2016369239,6.1337646058\H,3.008706448,-4.1329483526,6.4617297892\
H,6.2598999507,-3.5626233684,-0.3443977681\H,6.9136614821,-3.8184344608,1.2903492807\
H,5.4091903003,-4.6207967368,0.8077129593\H,3.45106296,1.0392100282,-2.8691331507\
H,2.581390574,1.6909000721,-1.4499363953\H,4.0689155692,2.4793258991,-2.005933972\
\Version=ES64L-G16RevB.01\State=1-A\HF=-1197.250468\RMSD=8.250e-09\RMSF=1.277e-
06\Dipole=-0.7961059,-3.9251149,1.2950532\Quadrupole=3.7445513,-11.7937462,8.0491949,-
8.2834092,0.8067622,0.7281352\PG=C01 [X(C16H29N1O3Si1)]\\@

Product H

HF=-1197.3118706 a.u. (0)
1\1\GINC-R02N13\FOpt\RB3LYP\6-31G(d,p)\C16H29N1O3Si1\WURTHWE\27-Apr-2023\0\\#
b3lyp/6-31G(d,p) Opt=readfc geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\Product H\\0,1\
C,1.7289118105,0.0757086183,-0.641946636\C,1.3338695846,-1.2637584069,0.0661858562\
C,0.1103085728,-1.9057922998,-0.596899556\N,-1.0492975034,-1.0332445386,-0.4673483101\
C,-0.7920383867,0.3041863678,-0.7721639526\C,0.441784042,0.8373355412,-0.8752267997\
C,2.6559197176,0.8972658272,0.2922731778\C,2.4880640574,-0.1845165625,-1.9705635117\
C,2.9561019672,1.1154172011,-2.6348897356\C,3.8628491524,1.9167936146,-1.6928435462\
C,3.1675934782,2.1915481515,-0.3536905138\O,-1.919666645,1.0647964811,-0.9273478539\
Si,-2.4566119985,2.1045355778,0.3110226361\C,-1.3686334703,3.632566443,0.3883774909\
C,-4.2048003874,2.5423518306,-0.1992859737\C,-2.401391427,1.1672627409,1.9357945863\
C,-2.2887850313,-1.6315649793,-0.9489202984\C,2.5032592241,-2.2187739707,0.1737984848\
O,3.3760628169,-2.1518947996,1.019344886\O,2.4952771973,-3.1572585744,-0.7940746546\
C,3.6015923926,-4.078767678,-0.7812138757\H,1.0641569574,-1.0085724631,1.0965429499\
H,0.3230625722,-2.126522981,-1.6536363596\H,-0.1238584284,-2.857442364,-0.1114177432\
H,0.496999552,1.8988654214,-1.0739442792\H,2.1148365892,1.1238830565,1.2187434502\
H,3.5138184885,0.2747179558,0.5696206679\H,1.8519416185,-0.754246551,-2.6551588375\
H,3.3733247936,-0.8019648173,-1.7660232875\H,3.4858886684,0.8831533426,-3.5658043912\
H,2.0841196943,1.7205267025,-2.9127585574\H,4.1696510794,2.858042613,-2.1634193014\
H,4.7810899771,1.3414591757,-1.5085431754\H,2.3343995887,2.8876976773,-0.5127764063\
H,3.8565163089,2.6932658988,0.3356369324\H,-1.3247856587,4.1359759041,-0.5828606956\
H,-0.3474336407,3.3756164213,0.6848516787\H,-1.764538716,4.3449426104,1.1207502316\
H,-4.2182349902,3.0264082578,-1.1811077776\H,-4.6565330091,3.232168424,0.5214490637\
H,-4.8345137678,1.6485763767,-0.2521745566\H,-1.3872242744,0.8113168458,2.1421171638\
H,-3.0659090653,0.2980966301,1.9156200158\H,-2.7084369441,1.8134906496,2.7649976476\
H,-2.4451455643,-2.5779961504,-0.4245688538\H,-3.128653673,-0.9719545626,-0.7407397594\
H,-2.2652044251,-1.8368752302,-2.0314258582\H,3.4272936674,-4.7576051592,-1.6143021343\
H,4.5435211754,-3.5425387362,-0.9139350016\H,3.6303572625,-4.6274645335,0.1622132739
\\Version=ES64L-G16RevB.01\State=1-A\HF=-1197.3118706\RMSD=3.929e-09\RMSF=1.314e-
06\Dipole=-0.7070982,-0.3899719,-0.2618372\Quadrupole=-0.9209574,7.6502282,-6.7292708,-
2.9390958,-7.8907882,5.3182845\PG=C01[X(C16H29N1O3Si1)]\\@

TPSS

2-Silyloxy-1-azabutadiene G

HF=-891.0724298 a.u. (0)
1\1\GINC-R01N44\FOpt\RTPSSTPSS\def2TZVP\C12H23N1O1Si1\WURTHWE\26-May-
2023\0\\# tpsstpss/def2tzvp opt=readfc geom=check guess=read freq pop=nbo emp=gd3bj
scrf=(solvent=dichloroethane)\\ 2-Silyloxy-1-azabutadiene G\\0,1\
C,-0.0400442138,-0.0923519179,0.0833688586\C,-0.059308501,-0.3001907394,1.6021906717\
C,1.3554342319,-0.1397373426,2.1958082167\C,2.3374046868,-1.0513317782,1.5043543019\
C,2.3720282179,-0.9093199183,0.0070710394\C,0.9534706999,-1.0469719777,-0.5880380858\
C,3.0411331748,-1.9539418554,2.2147154471\C,3.9887095172,-2.9548122329,1.7017963912\
O,3.9398383287,-4.1735749408,2.3437404205\Si,2.5733447288,-5.068872283,2.798537704\

C,3.2667166283,-6.7831019384,3.0799519039\N,4.8387919082,-2.726453695,0.7751966819\
C,5.6945720686,-3.8388200403,0.3597416412\C,1.8072800754,-4.4080111259,4.3785169539\
C,1.3378780688,-5.0320379547,1.3907057777\H,2.8703543096,-2.0086662601,3.2889402694\
H,1.3498048028,-0.3304487574,3.274265658\H,1.6752147581,0.9026753557,2.0450826556\
H,3.0597165753,-1.6344435853,-0.4311122143\H,2.7564365144,0.0928010769,-0.2367084388\
H,0.9950892517,-0.8623922125,-1.667773609\H,0.610855331,-2.0816201684,-0.4524143254\
H,-1.0446273772,-0.2388260153,-0.3313337152\H,0.2490712494,0.9455103001,-0.1353900351\
H,-0.4287036646,-1.3095883631,1.8288805439\H,-0.7423092447,0.4105651641,2.0816707499\
H,1.790433465,-5.3871745524,0.4576294866\H,0.9630099149,-4.0163589982,1.2235070224\
H,0.4786838785,-5.6753171515,1.6168546607\H,3.7307252771,-7.175776649,2.1681070682\
H,2.4726936943,-7.4763249998,3.3826377274\H,4.0252468353,-6.7751215927,3.8714261228\
H,1.2773397021,-3.4631949617,4.2186672055\H,2.5670218007,-4.2499859556,5.1529192859\
H,1.0822649765,-5.1354291524,4.765618534\H,6.2591297865,-3.5347155289,-0.5252781238\
H,6.4070203599,-4.1066349056,1.1513906237\H,5.1148890348,-4.7409235848,0.1240990138\\
Version=ES64L-G16RevB.01\State=1-A\HF=-891.0724298\RMSD=3.520e-09\RMSF=6.060e-
07\Dipole=-1.3163522,-0.3381819,0.358951\Quadrupole=-4.0099491,3.5521958,0.4577532,-
2.8569322,0.4455642,-0.5801726\PG=C01 [X(C12H23N1O1Si1)]\\@

Methyl acrylate

HF=-306.6537768 a.u. (0)
1\1\GINC-R03N46\FOpt\RTPSSTPSS\def2TZVP\C4H6O2\WURTHWE\21-Jun-2023\0\\#
tpsstpss/def2tzvp Opt=readfc geom=check guess=read emp=gd3bj Pop=NBO Freq
scrf=(solvent=dichloroethane)\\Methylacrylate)\\0,1\
C,0.0208563135,0.,0.0176628318\O,0.0131585819,0.,1.2387732425\
C,1.2209913413,0.,-0.8494799771\ C,2.4504036988,0.,-0.3282068993\
O,-1.1079864272,0.,-0.7347898307\C,-2.3487737881,0.,0.0178984275\
H,1.0491093637,0.,-1.9216893553\H,2.595695706,0.,0.7485236555\
H,3.3332765139,0.,-0.95920783\H,-3.1368933765,0.,-0.7334150994\
H,-2.4040813296,-0.8933737659,0.6437420224\H,-2.4040813296,0.8933737659,0.6437420224
\\Version=ES64L-G16RevB.01\State=1-A'\HF=-306.6537768\RMSD=8.896e-09\RMSF=4.510e-
06\Dipole=-0.116835,0.,-0.782647\Quadrupole=6.3118942,-2.1864667,-4.1254274,0.,
-1.4847024,0.\PG=CS [SG(C4H4O2),X(H2)]\\@

Van der Waals Complex

HF=-1197.7328322 a.u. (0)
1\1\GINC-R03N34\FOpt\RTPSSTPSS\def2TZVP\C16H29N1O3Si1\WURTHWE\27-Apr-
2023\0\\# tpsstpss/def2tzvp opt=readfc geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\ Van der Waals Complex \\0,1\
C,-0.301440291,0.0202061935,-0.2299023724\C,-0.2961554507,0.0137499089,1.3038419691\
C,1.1290892971,-0.1167421957,1.8544049348\C,2.0468644562,0.9874712762,1.2843056775\
C,2.0021543001,0.9761251834,-0.2213359877\C,0.6193313631,1.1295096233,-0.7867017942\
C,3.1362127287,0.7882299794,-0.9272317617\C,3.3180105899,0.7248626384,-2.3821050848\
N,2.3801327225,0.4791345754,-3.219367055\C,2.7339052494,0.4775354891,-4.6367811614\
O,4.595167842,0.9610442559,-2.82983105\Si,6.1214507996,1.0127042041,-2.1043473315\
C,6.4391744865,-0.5758527328,-1.1574367927\C,7.2728924336,1.140283359,-3.5731834474\
C,6.2924282379,2.5216418729,-1.0056335548\C,1.8292442914,3.994889758,-2.7802964816\
C,2.7530185263,4.1293450628,-1.8248171432\C,2.4686969451,4.5146290024,-0.428636419\
O,1.151506713,4.7278394154,-0.1897662257\C,0.8268280089,5.1268574251,1.1650670273\
O,3.3291401579,4.634994872,0.433018045\H,3.8034452402,3.9457188667,-2.0233740463\
H,0.7764919997,4.1659874409,-2.5813085773\H,2.1067283463,3.6979923956,-3.7864831428\
H,4.058712465,0.7106666748,-0.3555218416\H,3.0737065172,0.8653491621,1.6445787171\
H,1.681063726,1.9592146047,1.6467778079\H,0.6444451361,1.1091526493,-1.8758831739\
H,0.2231066933,2.1011928137,-0.4564551407\H,-1.3190763634,0.1684782005,-0.6096716605\
H,0.0459072777,-0.9520693047,-0.6037843531\H,-0.9216308386,-0.8039746485,1.6819639412\

H,-0.7390236411,0.9515360775,1.6689860594\H,1.5403855263,-1.0967337129,1.5779080205\
H,1.1268433354,-0.0624510674,2.9493289945\H,6.2387382647,-1.448975135,-1.7894227566\
H,5.8290635506,-0.6654958749,-0.2525191647\H,7.4924937981,-0.6169652665,-0.8527440599\
H,7.1802574172,0.2644069386,-4.2254310451\H,8.3160810519,1.206347849,-3.2412353194\
H,7.0518932204,2.0335704467,-4.1687732766\H,5.5342303905,2.562759132,-0.2171654226\
H,6.2158348905,3.4435196996,-1.5938432993\H,7.279089605,2.5171972081,-0.5251659936\
H,1.8365025447,0.2635271442,-5.2229014444\H,3.1428645231,1.4458156156,-4.9566372325\
H,3.4937601467,-0.282787029,-4.8637513331\H,-0.2577557117,5.2237928099,1.1794530383\
H,1.1596983048,4.3642450545,1.8723869956\H,1.3071922165,6.0796264084,1.3989614476\\
Version=ES64L-G16RevB.01\State=1-A\HF=-1197.7328322\RMSD=2.156e-09\RMSF=8.828e-
07\Dipole=-0.1592426,0.0597492,0.3755752\Quadrupole=5.6615299,-5.5478713,-0.1136586,-
7.8416301,-6.5295771,-3.0869642\PG=C01 [X(C16H29N1O3Si1)]\\@

TS-Diels-Alder

HF=-1197.7097369 a.u. (1, -239.6004 cm^{-1})
1\1\GINC-R03N14\FTS\RTPSSTPSS\def2TZVP\C16H29N1O3Si1\WURTHWE\28-Apr-
2023\0\\# tpsstpss/def2tzvp Opt=(ts,noeigentest,readfc) geom=check guess=read Pop=NBO Freq
emp=gd3bj scrf=(solvent=dichloroethane)\\ TS-Diels-Alder\\0,1\
C,0.0785990887,-0.3095893806,0.971145048\C,0.512161076,0.056672224,2.3941962532\
C,2.0385986386,0.2803145212,2.4717540638\C,2.7969011081,-0.8787109475,1.8907664289\
C,2.3895085473,-1.2492934314,0.490849425\C,0.8661884634,-1.5194379234,0.4597680494\
C,3.5707399016,-1.6572251669,2.6991838626\C,4.4804928261,-2.66088481,2.2454333208\
O,4.7685847817,-3.7209524315,3.0291870721\Si,3.7630607003,-4.4918713343,4.1824631658\
C,4.5670216345,-6.1690898297,4.349489581\N,5.1249500764,-2.5503010621,1.1028458848\
C,5.9723633882,-3.663590348,0.6694659172\C,3.823502804,-3.5543964157,5.8015518822\
C,2.0262971133,-4.6068484149,3.4967121658\C,5.832962903,-1.0649910699,0.5919687231\
C,5.2720756369,0.1777861738,1.0159437635\C,4.6086961634,1.0904074348,0.1646247464\
O,4.1503297448,2.2051607151,0.4767657722\O,4.4899523257,0.6453070824,-1.158207909\
C,3.8216878534,1.5609426758,-2.0413686266\H,5.4204756376,0.5203570029,2.0336384503\
H,5.8188677056,-1.219259813,-0.4840614353\H,6.8151307694,-1.2914931446,1.0142356194\
H,3.5852947129,-1.4527666984,3.7680377869\H,2.3503919708,0.4621966473,3.5054259255\
H,2.3021370255,1.1710688328,1.8824569927\H,2.9443876544,-2.1183406071,0.1348435488\
H,2.6048086428,-0.4217765141,-0.1916333793\H,0.5741222759,-1.7661185368,-0.5675844044\
H,0.639147362,-2.3963144706,1.0807575953\H,-0.9978407089,-0.5177707575,0.9468727986\
H,0.2570264068,0.5455900478,0.3043574596\H,0.2367935685,-0.7567276103,3.0791489098\
H,-0.0044556848,0.9596389342,2.7387667008\H,2.0268570301,-5.0619348803,2.4995265747\
H,1.5521187795,-3.6232374799,3.4235399897\H,1.4103604227,-5.2338860642,4.1531573582\
H,4.559450702,-6.7071244921,3.3948919177\H,4.0319814842,-6.7790025209,5.0870515079\
H,5.6075118813,-6.0754751137,4.6809765514\H,3.2951678438,-2.5966714238,5.7507489306\
H,4.8587632845,-3.360590737,6.1047915246\H,3.3502356521,-4.1531246696,6.5900075293\
H,6.284435135,-3.4684237937,-0.3592536701\H,6.8625767979,-3.7741046393,1.2993344174\
H,5.4021384504,-4.5936971547,0.7092497661\H,3.8083269665,1.0661875796,-3.0141803259\
H,2.7998004706,1.7587123573,-1.7026993005\H,4.3635136979,2.5094066029,-2.1047994708\\
Version=ES64L-G16RevB.01\State=1-A\HF=-1197.7097369\RMSD=3.469e-09\RMSF=1.313e-
06\Dipole=-0.725525,-3.7050695,1.2057848\Quadrupole=4.3810385,-13.2950406,8.9140021,-
7.6742818,0.7097126,0.8384025\PG=C01 [X(C16H29N1O3Si1)]\\@

Product H

HF=-1197.7600269 a.u. (0)
1\1\GINC-R03N44\FOpt\RTPSSTPSS\def2TZVP\C16H29N1O3Si1\WURTHWE\27-Apr-
2023\0\\# tpsstpss/def2tzvp opt=readfc geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\ Product H\\0,1\
C,0.404027183,-0.1939585215,0.2621011915\C,0.9111253219,-0.3133294472,1.7049364655\
C,2.372122717,0.1419505691,1.8134724276\C,2.5619852408,1.5562048709,1.2483784629\
C,2.0622154374,1.6903620703,-0.2134572017\C,0.5799890033,1.2379108676,-0.2568694735\

C,2.9366472421,0.8562327342,-1.1224541559\C,3.4775960538,1.2978059567,-2.2790636198\
N,3.2632994368,2.5643341487,-2.8128323318\C,2.1434963384,3.282509489,-2.2093304134\
C,2.2232481277,3.1768643682,-0.6818883554\C,1.2511487223,4.1058673244,0.0118602462\
O,0.1519644033,4.3578034078,-0.738402368\C,-0.839416942,5.2173616437,-0.1172950549\
O,4.3332537814,0.525698252,-3.0259277162\Si,5.8948971295,0.1434043187,-2.4946507188\
C,5.8517711626,-1.2380319398,-1.2266274525\C,6.760940948,-0.4201695601,-4.0541874641\
C,6.6666572992,1.6859741835,-1.7631444834\C,3.3876468708,2.7562193774,-4.257511738\
O,1.4124427233,4.5803951229,1.1240993997\H,3.2229048222,3.4978746943,-0.3671955426\
H,1.1819166792,2.886311231,-2.5701372916\H,2.2095325129,4.3288131583,-2.5218212128\
H,3.226650168,-0.1337149099,-0.7927107826\H,3.6197735199,1.8451276823,1.2899339074\
H,2.0069602158,2.2665481173,1.8738085206\H,0.1960761041,1.325767917,-1.2791984397\
H,-0.0171799375,1.9106872388,0.3761976801\H,-0.653401839,-0.478830708,0.2055693854\
H,0.9570870153,-0.8889005679,-0.3837459562\H,0.8063263491,-1.3441049263,2.0646317936\
H,0.288355558,0.3185880289,2.3547740999\H,3.0148634059,-0.5677218097,1.2759099873\
H,2.6986509957,0.1239215226,2.8603435115\H,5.2733825508,-2.0945294842,-1.5922804587\
H,5.4119885652,-0.9063299498,-0.2798229672\H,6.8715535703,-1.5857625688,-1.0176165816\
H,6.2506067953,-1.2837626184,-4.4966250853\H,7.7943792711,-0.7163184253,-3.8376932466\
H,6.7877846683,0.379714257,-4.8029731198\H,6.0686510121,2.0566400946,-0.9223717817\
H,6.7397441152,2.4866354726,-2.507702806\H,7.6760906009,1.473960033,-1.390354452\
H,2.5366460876,2.3245254218,-4.8094276465\H,3.422938695,3.8309770378,-4.4555673312\
H,4.3079882413,2.2957620651,-4.6135109155\H,-1.639675621,5.3022072843,-0.8508517801\
H,-1.2010472536,4.7601297337,0.806206399\H,-0.4018467645,6.1938991545,0.100191663
\\Version=ES64L-G16RevB.01\State=1-A\HF=-1197.7600269\RMSD=4.695e-09\RMSF=1.289e-
06\Dipole=-0.0549439,0.0874132,-0.8802475\Quadrupole=8.1848902,-1.5235736,-6.6613166,-
6.5980134,-1.121396,-7.2677308\PG=C01 [X(C16H29N1O3Si1)]\\@

PBE1PBE
2-Silyloxy-1-azabutadiene G
HF=-890.094248 a.u. (0)
1\1\GINC-R04N05\FOpt\RPBE1PBE\def2TZVP\C12H23N1O1Si1\WURTHWE\27-Apr-
2023\0\\# pbe1pbe/def2tzvp opt=readfc geom=check guess=read freq pop=nbo emp=gd3bj
scrf=(solvent=dichloroethane)\\ 2-Silyloxy-1-azabutadiene G \\0,1\
C,-0.3693523978,-0.0595752295,-0.0482294658\C,-0.1627198288,0.0379093113,1.4295190715\
C,1.2608420904,0.2817191654,1.8248303705\C,2.171407603,-0.7981065558,1.2357987981\
C,1.9917779935,-0.9106008161,-0.2709923198\C,0.5339499403,-1.1434108842,-0.6401365283\
C,-1.1186333295,-0.1005270309,2.3532085429\C,-2.5478025119,-0.3456049572,2.1163228778\
O,-3.3852947188,0.400722865,2.8769886388\N,-2.9793741244,-1.2224385471,1.3102514665\
C,-4.4131893789,-1.3445867244,1.1618269405\H,1.3582263186,0.323087836,2.9122188829\
H,1.5758869091,1.2563078301,1.4286951242\H, 1.9295557783,-1.7591291534,1.7039922067\
H,3.2132790316,-0.5768576367,1.4836805567\H,2.6157739829,-1.717922928,-0.6652166184\
H,2.3391275239,0.0158277723,-0.7451009101\H,0.2099529723,-2.1189089612,-0.2603456156\
H,0.4130760591,-1.168913086,-1.7266603849\H,-1.4138783353,-0.2542977525,-0.2836748598\
H,-0.0879317982,0.9045905448,-0.4937335067\H,-0.8533530029,0.035727193,3.3987090077\
Si,-3.3639472028,2.0731178091,3.0840546581\H,-4.632578613,-2.0723276661,0.3798305312\
H,-4.8856403641,-0.3926592606,0.8944182543\H,-4.8873122858,-1.6852259666,2.0890236031\
C,-5.0582323783,2.4489212398,3.750207287\C,-2.0509284331,2.5848616802,4.3037882723\
C,-3.0727406667,2.854897221,1.4186332501\H,-3.0993499266,3.9450495834,1.4981016556\
H,-2.096468951,2.5692999496,1.0186711897\H,-3.8396977496,2.5474334233,0.7032259558\
H,-5.171594068,3.5222778609,3.9239662096\H,-5.8332724167,2.1329488675,3.047901592\
H,-5.2254975945,1.9336653274,4.699456631\H,-2.181435589,3.6408078665,4.5585708745\
H,-2.1256975612,2.0048958089,5.2272706203\H,-1.046103815,2.4579059802,3.8961948526
\\Version=ES64L-G16RevB.01\State=1-A\HF=-890.094248\RMSD=3.376e-09\RMSF=3.229e-
06\Dipole=0.4331303,1.261236,0.1991315\Quadrupole=2.9213238,-2.7432324,-0.1780914,-
2.6257249,-0.9950367,0.6755765\PG=C01 [X(C12H23N1O1Si1)]\\@

Methyl acrylate
HF=-306.2510928 a.u. (0)
1\1\GINC-R02N20\FOpt\RPBE1PBE\def2TZVP\C4H6O2\WURTHWE\21-Jun-2023\0\\#
pbe1pbe/def2tzvp Opt=readfc geom=check guess=read emp=gd3bj Pop=NBO Freq
scrf=(solvent=dichloroethane)\\methyl acrylate)\\0,1\
C,0.0158423186,0.,0.0153163324\O,0.0189374757,0.,1.2232311363\
C,1.2129643671,0.,-0.8497799473\ C,2.4318531345,0.,-0.3269507625\
O,-1.1001135621,0.,-0.7184585218\C,-2.3241536347,0.,0.0134733878\
H,1.0437861289,0.,-1.9200766967\ H,2.5694356872,0.,0.7486770503\
H,3.3152599836,0.,-0.9533532746\ H,-3.1158090914,0.,-0.7313353605\
H,-2.3931637696,-0.8887982566,0.6414049335\H,-2.3931637696,0.8887982566,0.6414049335
\\Version=ES64L-G16 RevB.01\State=1-A'\HF=-306.2510928\RMSD=3.501e-09\RMSF=1.750e-
05\Dipole=-0.106331,0., -0.802583\ Quadrupole= 6.2924609,-2.2405274,-4.0519335,0.,-
1.4425267,0.\PG=CS [SG(C4H4O2),X(H2)]\\@

Van der Waals Complex
HF=-1196.3528604 a.u. (0)
1\1\GINC-R03N34\FOpt\RPBE1PBE\def2TZVP\C16H29N1O3Si1\WURTHWE\28-May-
2023\0\\# pbe1pbe/def2tzvp opt=readfc geom=check guess=read freq pop=nbo emp=gd3bj
scrf=(solvent=dichloroethane)\\ Van der Waals Complex\\0,1\
H,-3.9266130606,0.9497163069,-2.5277426913\C,-3.2555702465,1.3168984631,-1.7462729858\
C,-4.0350382079,2.0573448854,-0.6708505504\C,-3.1135255654,2.5207209374,0.4459561484\
C,-2.3160983346,1.3623276825,1.0486686505\C,-1.6006243743,0.593147207,-0.0139609584\
C,-2.4727285978,0.1486631751,-1.1491180755\C,-0.2902177974,0.3189694511,-0.0351536886\
C,0.7434355656,0.6438299451,0.9515851094\O,2.0117373153,0.6086084328,0.4858070036\
Si,2.6776217664,0.8855594297,-1.0317276357\C,1.9290618027,2.4329042096,-1.7495291145\
N,0.5072969366,0.892046,2.1742041451\C,1.637513833,1.1815704992,3.0245516637\
H,1.2814499686,1.4271528096,4.025974113\C,4.4874399534,1.0989141537,-0.6632442591\
C,2.4178218738,-0.5808676494,-2.1583064184\C,-0.468287104,-2.2032086155,2.890469594\
C,-1.1244935172,-2.5497632318,1.7916320671\C,-0.3991064847,-2.8953255548,0.5565047343\
O,0.8015880369,-2.957993068,0.4337033025\O,-1.2518328997,-3.1403123682,-0.4446460912\
C,-0.6587118206,-3.4619953935,-1.6985854083\H,0.0852204013,-0.2200233856,-0.8992613062\
H,-2.2068152465,-2.5680677642,1.7455729532\H,-0.9903081386,-1.9274871948,3.7980542913\
H,0.6150266135,-2.176728077,2.899297266\H,-3.1889736383,-0.5888578136,-0.762476009\
H,-1.8772531804,-0.3546260296,-1.9143023978\H,-2.5539428284,2.0082052172,-2.2278272143\
H,-4.8003595554,1.3896565723,-0.255853255\H,-4.5638479163,2.9105820009,-1.1055406699\
H,-3.6848063508,3.0164711586,1.2356686909\H,-2.4120162352,3.2646464649,0.0501777505\
H,-3.0152050591,0.6755616725,1.5461708454\H,-1.6145039935,1.7052457394,1.805825284 9\
H,-0.010051298,-2.6522594391,-2.034765151\H,-1.4839372553,-3.5986942263,-2.3929821052\
H,-0.0716162744,-4.3778702452,-1.6217363786\H,2.2346144029,2.0222084851,2.6522333817\
H,2.3161275897,0.3240245026,3.1029172423\H,3.1720454726,-0.5679586653,-2.9504159583\
H,2.5216878093,-1.5180332186,-1.6057550727\H,1.4368246908,-0.5710368306,-2.6385502229\
H,5.0443015813,1.3032522525,-1.58153777\H,4.649845369,1.9300755293,0.0271144983\
H,4.8999486029,0.193186647,-0.2115442302\H,2.3936803632,2.665331301,-2.7118726349\
H,0.854985993,2.3145512493,-1.911379649\H,2.0832403934,3.2854804542,-1.0832681354
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06\Dipole=-0.6788242,0.2941757,-1.2858491\Quadrupole=1.9891441,-
4.5526107,2.5634667,4.6643817,-2.2136789,1.4766129\PG=C01 [X(C16H29N1O3Si1)]\\@

TS-C..N
HF=-1196.3288379 a.u. (1, -292.4280cm^{-1})
1\1\GINC-R03N04\FTS\RPBE1PBE\def2TZVP\C16H29N1O3Si1\WURTHWE\29-Apr-202
3\0\\# pbe1pbe/def2tzvp Opt=(ts,noeigentest,readfc,maxstep=2) geom=check guess=read
Pop=NBO Freq emp=gd3bj scrf=(solvent=dichloroethane)\\ TS-C..N \\0,1\

C,0.0794176924,-0.3894365128,1.0377786857\C,0.5052006452,-0.0407955543,2.4546556041\
C,2.0123200793,0.1923051238,2.5344503536\C,2.7945894242,-0.9393338848,1.9487643609\
C,2.3615336128,-1.3655819256,0.5833328848\C,0.8500456898,-1.5948127977,0.5254311443\
C,3.7654167528,-1.5271712542,2.6589934054\C,4.6172005082,-2.6045253643,2.1901978324\
O,4.7463406327,-3.68194277,2.9501654343\Si,3.6713844567,-4.3850769102,4.072749997\
C,4.5002516645,-6.0061384989,4.4307352823\N,5.284534419,-2.545295094,1.0888235867\
C,6.0274087689,-3.709993214,0.6589841606\C,3.5513463857,-3.3358753529,5.6037528112\
C,2.0234583548,-4.6044661728,3.2427365172\C,6.0355448826,-1.0926470742,0.4319392574\
C,5.6600994459,0.1734893492,0.9125198283\C,4.8120996553,1.0693462033,0.2327431302\
O,4.4238288324,2.166968225,0.6369722306\O,4.4317331264,0.6422161103,-1.020483671\
C,3.5967187993,1.5263682461,-1.739113624\H,5.9896135984,0.5015048981,1.8905062064\
H,5.8312910944,-1.2768656117,-0.6182334721\H,7.0309953425,-1.4331703609,0.7167178365\
H,3.9363953981,-1.218742069,3.6858507453\H,2.3283064296,0.380798424,3.5627834481\
H,2.2676243208,1.0870746948,1.950665256\H,2.9019029422,-2.2550025658,0.2599486491\
H,2.6260142292,-0.5696735875,-0.1193058133\H,0.5647939222,-1.8268778821,-0.5040972663\
H,0.5910827777,-2.4727820281,1.1282338554\H,-0.9961501398,-0.5841384004,1.0019843604\
H,0.2684796083,0.4684430737,0.3807919611\H,0.2310936309,-0.8611855101,3.1283681401\
H,-0.0203578842,0.8493874655,2.809904934\H,2.129530273,-5.1334045584,2.2924714479\
H,1.5429172098,-3.6430626393,3.0535755358\H,1.3633275374,-5.1927913795,3.8861622912\
H,4.6093542428,-6.5991737849,3.5196919624\H,3.9076852104,-6.5840333598,5.1447322604\
H,5.4925088377,-5.8508053968,4.8611895548\H,2.9480019873,-2.4404119426,5.4448575046\
H,4.5418591825,-3.0323436655,5.9516461362\H,3.0812674692,-3.92016819,6.4003447729\
H,6.3766570749,-3.5374135443,-0.3594127984\H,6.8935001369,-3.9000046722,1.2989226095\
H,5.3922107489,-4.5954373259,0.6753076446\H,3.4037542438,1.0466951903,-2.6983305637\
H,2.6505992604,1.6982333497,-1.2188491123\H,4.079468198,2.4924756458,-1.9004128392
\\Version=ES64L-G16RevB.01\State=1-A\HF=-1196.3288379\RMSD=4.245e-09\RMSF=9.297e-
07\Dipole=-1.1968298,-4.1934475,1.321979\Quadrupole=4.0371358,-13.5396897,9.5025539,-
11.1288994,1.9173503,1.2126521\PG=C01[X(C16H29N1O3Si1)]\\@

Dipolar Intermediate

HF=-1196.3415293 a.u. (0)
1\1\GINC-R10N27\FOpt\RPBE1PBE\def2TZVP\C16H29N1O3Si1\WURTHWE\31-May-
2023\0\\# pbe1pbe/def2tzvp opt=(maxstep=3) geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\ Dipolar Intermediate \\0,1\
H,-1.932864647,3.1729792616,2.3981674418\C,-2.2419698457,2.6521109779,1.4887457553\
C,-0.9940134728,2.1873784542,0.7334214631\C,-1.3582054757,1.5677385399,-0.5773222953\
C,-2.2593621305,2.3984485805,-1.4347409047\C,-3.5023847918,2.8490206707,-0.6675937875\
C,-3.1224111542,3.5444162508,0.6296386101\C,-0.9823250781,0.3464236242,-0.975751617\
C,-0.1687018595,-0.5954191214,-0.214758135\O,-0.6387757481,-1.7982623947,0.0018852521\
Si,-2.2320919338,-2.4323055464,0.0172224678\C,-1.9397445421,-4.1397650848,0.6743105869\
N,1.0236963422,-0.3451647453,0.2283217817\C,1.8549805347,0.850165746,-0.1838735221\
C,3.1156968763,0.4669961464,-0.8233247839\C,4.2845645393,0.3963087894,-0.0803701701\
O,4.4361752108,0.5938481859,1.1405100374\C,1.7073770477,-1.335368141,1.048950368\
H,1.911272133,-2.2409677432,0.4776757725\O,5.3947782803,0.0619314405,-0.8438689248\
C,6.6079331122,-0.0537611213,-0.1358316029\C,-3.2573042445,-1.3909816741,1.1620346858\
C,-2.9105259918,-2.4686339152,-1.7120627155\H,-1.3689757905,-0.0540050291,-1.9078992735\
H,3.1298991778,0.2183394779,-1.8766855417\H,2.038844067,1.4006242998,0.7417479361\
H,1.2051149641,1.4430266885,-0.8245450649\H,-0.4092229341,1.5052914599,1.3505517575\
H,-0.3605960781,3.0603813485,0.5302677628\H,-2.8134136034,1.7736429311,1.807943583\
H,-4.0213190912,3.8291728765,1.1829539332\H,-2.5853954584,4.4724218037,0.3996114653\
H,-4.099871734,3.5090910331,-1.3011613286\H,-4.1245864413,1.9741938722,-0.4463126609\
H,-1.6987879476,3.2905983729,-1.743257944\H,-2.5309415247,1.8558035083,-2.3422976227\
H,7.3697501015,-0.2990242232,-0.8767030063\H,6.5662771579,-0.8468719834,0.6163160752\

H,6.8773768772,0.8782294788,0.3676480415\H,1.0783655623,-1.5946225169,1.9007416681\
H,2.6445813456,-0.8943591173,1.3806184379\H,-2.177591222,-2.8719718361,-2.414895789\
H,-3.224005132,-1.4824656847,-2.0587362577\H,-3.7873863212,-3.1225471144,-1.731544772\
H,-3.4447553639,-0.4005750706,0.7443115912\H,-2.7694603044,-1.2744197076,2.1326755862\
H,-4.2233480192,-1.8769320957,1.3251794214\H,-1.2768667063,-4.7029162793,0.0131242767\
H,-2.8859757211,-4.681759037,0.7487040795\H,-1.4873450997,-4.1046014273,1.6679631783
\\Version=ES64L-G16RevB.01\State=1-A\HF=-1196.3415293\RMSD=6.290e-09\RMSF=5.435e-
06\Dipole=-6.5771337,-0.9840076,-0.2129633\Quadrupole=-20.9822936,16.8283089,4.1539847,-
5.4349228,-0.5192771,-1.5951829\PG=C01 [X(C16H29N1O3Si1)]\\@

TS-C..C

HF=-1196.3348037 a.u (1, -52.2241cm^{-1})
1\1\GINC-R03N28\FTS\RPBE1PBE\def2TZVP\C16H29N1O3Si1\WURTHWE\08-Jun-2023\0\\#
pbe1pbe/def2tzvp Opt=(ts,noeigentest,readfc,maxstep=4) geom=check guess=read nosym
emp=gd3bj freq pop=nbo scrf=(solvent=dichloroethane)\\TS-C..C\\0,1\
H,0.002167473,-0.0026576373,-0.0065547751\C,0.0001232439,-0.0005849808,1.0867427682\
C,1.4500023842,0.0019013524,1.5866150407\C,1.4584114892,-0.0357302402,3.0825700708\
C,0.6981208614,-1.1830443855,3.6666454856\C,-0.7396768335,-1.2220092288,3.1444552388\
C,-0.7740065316,-1.1924770206,1.6250393202\C,1.8668062504,0.9677818454,3.8844969437\
C,2.7047445185,2.0587062037,3.5019438102\O,2.5537218257,3.2305349751,4.0881778755\
Si,1.2006928985,3.9097480708,4.8736387214\C,1.6765306576,5.7001488087,4.9746818826\
N,3.649025723,1.9798292642,2.5967740547\C,4.4887177769,0.7384096282,2.2592149574\
C,4.2372167234,-0.5354673777,2.9204877689\C,4.3720152199,-0.6205902625,4.2972440979\
O,4.6360580436,0.3156968248,5.0699346763\C,4.3114997394,3.202566194,2.1818554309\
H,3.5818418107,3.9960458305,2.0376918161\O,4.1272869772,-1.8799344856,4.8120684188\
C,4.1691984986,-1.9772349679,6.2182260679\C,-0.3003702107,3.6397003885,3.8109408619\
C,1.0190263015,3.1667229473,6.5686784806\H,1.6166812233,0.9341349767,4.9385270506\
H,3.9090711358,-1.3910554683,2.3496596797\H,5.4847339281,1.1277864261,2.5048706428\
H,4.4309847956,0.6500026334,1.1722635426\H,1.9792014486,0.8723869464,1.2034865648\
H,1.9524355653,-0.8894505291,1.1991180366\H,-0.4901979843,0.9276711719,1.4018815256\
H,-1.8084670644,-1.1637506664,1.2712317445\H,-0.3315925792,-2.1166468936,1.2338339068\
H,-1.2430116576,-2.1135902793,3.5275068551\H,-1.2833672844,-0.3554426431,3.5379508503\
H,1.2093644243,-2.1067284117,3.3702373929\H,0.7177524737,-1.138460748,4.7572315585\
H,3.9402803733,-3.0156836289,6.4584984461\H,3.4316172709,-1.3224237979,6.69025197\
H,5.1554157689,-1.7211488504,6.6143912543\H,4.8233333647,3.0044128755,1.2402415461\
H,5.0465638217,3.5308467333,2.9210855305\H,1.9840465758,3.1251960551,7.0795324387\
H,0.5964007219,2.1606754911,6.5443018731\H,0.3499240183,3.7947317738,7.1641361985\
H,-0.5679835822,2.5833107833,3.75095933\H,-0.1326207143,4.0124552196,2.7973805372\
H,-1.1492127798,4.1837548998,4.2348122469\H,2.5994607908,5.8250944517,5.5460891547\
H,0.8897554185,6.2739605121,5.4711768481\H,1.8288486278,6.1216299471,3.9783023549
\\Version=ES64L-G16RevB.01\HF=-1196.3348037\RMSD=3.409e-09\RMSF=2.266e-
06\Dipole=-2.8863773,2.1873467,-1.1733159\Quadrupole=-21.5467343,23.463972,-
1.9172377,10.5842777,-32.2769596,13.7449679\PG=C01 [X(C16H29N1O3Si1)]\\@

Product H

HF=-1196.3980578 a.u. (0)
1\1\GINC-R01N25\FOpt\RPBE1PBE\def2TZVP\C16H29N1O3Si1\WURTHWE\28-Apr-
2023\0\\# pbe1pbe/def2tzvp opt=readfc geom=check guess=read Pop=NBO Freq emp=gd3bj
scrf=(solvent=dichloroethane)\\Product H\\0,1\
C,0.3943028959,-0.1880994083,0.2529938062\C,0.8926338063,-0.3145589769,1.6851438171\
C,2.3441041587,0.1277357423,1.8012760879\C,2.5479646954,1.5287193048,1.2410238301\
C,2.0570996449,1.6764545432,-0.210356308\C,0.5852985763,1.2298011594,-0.2638575549\
C,2.9272995369,0.8496548806,-1.1172040716\C,3.4806479978,1.2925143603,-2.2578571917\
N,3.278040743,2.55756271,-2.7760499805\C,2.1743190211,3.2721004245,-2.1799140732\
C,2.2244795057,3.1514249052,-0.6643784582\C,1.2519266864,4.076759899,0.0167787294\

O,0.1835302386,4.3487604744,-0.7350383142\C,-0.7980959757,5.1967640216,-0.1424173703\
O,4.3221873779,0.5272707149,-2.9921143349\Si,5.888085446,0.1644780727,-2.4979905642\
C,5.8744141186,-1.1645788359,-1.190790965\C,6.7110913354,-0.4460809485,-4.049811072\
C,6.6718130114,1.7219173427,-1.8428109079\C,3.4068783969,2.7594195659,-4.201355428\
O,1.4023550148,4.5301637141,1.1256886311\H,3.2167335918,3.4708078038,-0.331383809 \
H,1.2130653232,2.898021805,-2.5601567424\H,2.249812134,4.3210662577,-2.4748701182\
H,3.2020940144,-0.1471947112,-0.8034177174\H,3.6059952253,1.8068064351,1.2868705179\
H,2.0046492635,2.2428108089,1.8681538506\H,0.2080516605,1.3181354046,-1.285841278\
H,-0.0163550288,1.9032528278,0.3602091325\H,-0.6632177784,-0.4611968006,0.1930476257\
H,0.9354852184,-0.8906368247,-0.3904966066\H,0.7779083025,-1.3422136325,2.0423496862\
H,0.2723498184,0.3163672005,2.334378491\H,2.9848605727,-0.5872159523,1.2733602334\
H,2.664290647,0.1068417441,2.8471874393\ H,5.2955296745,-2.0319032984,-1.518412579\
H,5.4497351612,-0.8005212906,-0.2526718406\H,6.8972297805,-1.4971642213,-0.9906309386\
H,6.1941622247,-1.3248714906,-4.4436655965\H,7.7481231188,-0.7270288612,-3.847975565\
H,6.7120963249,0.3257489756,-4.8233100711\H,6.0995949506,2.1148848097,-0.9983353488\
H,6.7188659633,2.4952103087,-2.6132106822\H,7.689326583,1.5206414713,-1.4970008686\
H,2.5553054646,2.3455562403,-4.7618754863\H,3.4557333714,3.8317463888,-4.397763765\
H,4.3188553825,2.2967024675,-4.5692596217\H,-1.5835523691,5.3053958229,-0.8859866709\
H,-1.1950101414,4.7429594148,0.766217711\H,-0.3673363819,6.1683306436,0.1006975068
\\Version=ES64L-G16 RevB.01\State=1-A\HF=-1196.3980578\RMSD=6.949e-09\RMSF=1.030e-
06\Dipole=0.0241349,0.0692151,-0.9170283\Quadrupole=8.3336504,-1.3688935,-6.9647569,-
6.5677954,-1.1686811,-7.2370345\PG=C01 [X(C16H29N1O3Si1)]\\@

wB97X-D

2-Silyloxy-1-azabutadiene G
HF=-890.7220245 a.u. (0)
1\1\GINC-R03N46\FOpt\RwB97XD\def2TZVP\C12H23N1O1Si1\WURTHWE\02-Jun-2023\0\\#
wb97xd/def2tzvp opt=readfc geom=check guess=read freq pop=nbo scrf=(solvent=dichloroethane)\\
2-Silyloxy-1-azabutadiene G)\\0,1\
C,-0.1157432857,-0.1548591947,0.3152843718\C,0.0414112552,-0.1932844074,1.8315098607\
C,1.5099272659,-0.0364291842,2.2362538814\C,2.3828006171,-1.0504247892,1.547519768\
C,2.2297282935,-1.0821110125,0.0533481016\C,0.7558649805,-1.214243087,-0.3496813106 \
C,3.1676144103,-1.861277837,2.258387504\C,4.0482368873,-2.9275137199,1.7448892846\
O,3.9715581622,-4.0941678034,2.4328030384\Si,2.5951591918,-5.033104276,2.6760585224\
C,3.2625927007,-6.6799732601,3.2186376398\N,4.8539287398,-2.7646944631,0.7837505333\
C,5.649302715,-3.905638802,0.3693373676\C,1.5045773993,-4.2882524694,3.9905007763\
C,1.6951052806,-5.1315871542,1.0482535956\H,3.1363646322,-1.7979330194,3.3421881521\
H,1.6227433146,-0.1077134005,3.3191576106\H,1.8461098893,0.9643700372,1.9395116576\
H,2.8257682208,-1.8814220559,-0.3813619043\H,2.6196310063,-0.1397058942,-0.3489787409\
H,0.671723571,-1.1530024235,-1.4365286875\H,0.3934427428,-2.206512362,-0.061030966\
H,-1.1623915517,-0.3009249397,0.0396486862\H,0.1745014315,0.8357057487,-0.0520208728\
H,-0.3338956648,-1.1494861887,2.2113501228\H,-0.5548837334,0.5922429796,2.300012886\
H,2.3269182479,-5.5744311779,0.2754663977\H,1.3966468663,-4.1351202147,0.7141055482\
H,0.7918418023,-5.7388875366,1.1399921599\H,3.9167555965,-7.1072333064,2.4562240779\
H,2.444611156,-7.3814391208,3.3981042311\H,3.8329568263,-6.5832988633,4.144773916\
H,1.0577041347,-3.3512699359,3.6540455581\H,2.0690044606,-4.0912531741,4.9044728631\
H,0.6960832714,-4.9816784207,4.2361671696\H,6.21959093,-3.6380884908,-0.5193905441\
H,6.3530802464,-4.2085597202,1.1504883763\H,5.0302388411,-4.7777182987,0.1360934573
\\Version=ES64L-G16RevB.01\State=1-A\HF=-890.7220245\RMSD=3.906e-09\RMSF=1.294e-
06\Dipole=-1.3396005,-0.4397197,0.3511487\Quadrupole=-4.3128949,4.1179929,0.194902,-
3.081276,0.7088866,-0.0351551\PG=C01 [X(C12H23N1O1Si1)]\\@

Methyl acrylate
HF=-306.4944189 a.u. (0)
1\1\GINC-R08N43\FOpt\RwB97XD\def2TZVP\C4H6O2\WURTHWE\21-Jun-2023\0\\#wb97xd/def2tzvp Opt=readfc geom=check guess=read Pop=NBO Freq scrf=(solvent=dichloroethane)**Fehler! Linkreferenz ungültig.**)\\0,1\
C,0.0165653325,0.,0.0214305452\O,0.0236183004,0.,1.2284791057\
C,1.217857821,0.,-0.8470321165\ C,2.436895482,0.,-0.3295563239\
O,-1.0998708906,0.,-0.7090655033\C,-2.3316482913,0.,0.0135928355\
H,1.0474295604,0.,-1.9158856531\H,2.5839570506,0.,0.7438279535\
H,3.3152289678,0.,-0.9614746723\H,-3.1151988969,0.,-0.7383153555\
H,-2.4065795838,-0.8890989716,0.6387761977\H,-2.4065795838,0.8890989716,0.6387761977
\\Version=ES64L-G16RevB.01\State=1-A'\HF=-306.4944189\RMSD=6.181e-09\RMSF=1.450e-05\Dipole=-0.1240524,0.,-0.8118965\Quadrupole=6.395939,-2.2346709,-4.1612681,0.,-1.4490501,0.\PG=CS [SG(C4H4O2),X(H2)]\\@

Van der Waals Complex
HF=-1197.2226717 a.u (0)
1\1\GINC-R01N27\FOpt\RwB97XD\def2TZVP\C16H29N1O3Si1\WURTHWE\02-Jun-2023\0\\#wb97xd/def2tzvp opt=readfc geom=check guess=read Pop=NBO Freq scrf=(solvent=dichloroethane)\\ Van der Waals Complex\\0,1\
C,-0.347088653,0.2109510344,-0.2249448731\C,-0.3694547697,0.2320736546,1.3006000481\
C,1.0187405474,-0.0257189349,1.8782371654\C,2.0508714349,0.9544479153,1.3090007431\
C,2.0356192029,0.9338890361,-0.1945156259\C,0.6815845486,1.2024541291,-0.7816866207\
C,3.1554771429,0.6750577007,-0.87421627\C,3.3465512485,0.6275745297,-2.3351947563\
N,2.4484786598,0.2526003063,-3.1467830767\C,2.7664675316,0.2785314946,-4.5601647845\
O,4.5575385738,1.0272954334,-2.7798005444\Si,6.1112568453,1.1015701321,-2.1485455861\
C,6.5357678994,-0.5269596329,-1.346348371\C,7.1746379446,1.3952864632,-3.6446170789\
C,6.2634313757,2.5181596544,-0.947841806\C,1.9720216103,3.8702483853,-2.7511147674\
C,2.8391346781,3.9745044382,-1.7554878341\C,2.4855027487,4.3500407649,-0.3701270225\
O,1.1969123766,4.6569627247,-0.2141459172\C,0.7807345573,5.0102058849,1.1036058402\
O,3.285689942,4.3742760482,0.5356416259\H,3.8882339286,3.7516261647,-1.8939934733\
H,0.9180011501,4.0711280581,-2.6111469284\H,2.2977508481,3.5645238557,-3.7369763263\
H,4.0602014362,0.529488247,-0.2940016371\H,3.0482980569,0.7305366425,1.6902021179\
H,1.7970344548,1.9667014671,1.6449477422\H,0.7138428951,1.1620176289,-1.8660392351\
H,0.3822521418,2.2138752848,-0.4831198266\H,-1.3351049968,0.4500919218,-0.6236379224\
H,-0.0968895543,-0.7960468585,-0.5738704029\H,-1.0773082485,-0.5085256901,1.6793786983\
H,-0.723230929,1.2122497085,1.6398542683\H,1.3289319589,-1.047033051,1.6347774708\
H,1.0011861085,0.0514477816,2.9673161531\H,6.3400457961,-1.3552530284,-2.0307393453\
H,5.9769622446,-0.7059967164,-0.4265216582\H,7.5995828407,-0.541847618,-1.0962820601\
H,7.0989248722,0.5651112776,-4.3495789055\H,8.2221247352,1.4984250128,-3.351697864\
H,6.8763852509,2.3108150168,-4.1596084085\H,5.4914107085,2.4984212673,-0.1767532487\
H,6.1971596322,3.4775385321,-1.4656934322\H,7.2379518886,2.4766286757,-0.4545804767\
H,1.9051829453,-0.0742708008,-5.1266023238\H,3.0162210623,1.2876152027,-4.9045664622\
H,3.6226865086,-0.3607489283,-4.7984596869\H,-0.2813026149,5.224904605,1.0298757767\
H,0.9505362321,4.1837443607,1.7936920364\H,1.3217562425,5.8884851386,1.4538116015
\\Version=ES64L-G16RevB.01\State=1-A\HF=-1197.2226717\RMSD=3.694e-09\RMSF=1.076e-06\Dipole=-0.0320444,0.3072481,0.2299585\Quadrupole=6.5486155,-5.7761647,-0.7724509,-8.3724917,-6.9233109,-2.9780033\PG=C01 [X(C16H29N1O3Si1)]\\@

TS-C..N
HF=-1197.195086 a.u (1, -355.0828 cm^{-1})

1\1\GINC-R07N15\FTS\RwB97XD\def2TZVP\C16H29N1O3Si1\WURTHWE\04-Jun-2023\0\\#
wb97xd/def2tzvp Opt=(ts,noeigentest,calcfc,maxstep=2) geom=check guess=read Pop=NBO Freq
scrf=(solvent=dichloroethane)\\ TS-C..N \\0,1\
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C,-0.154429225,-0.0251167887,0.6121730588\C,-0.8770406738,-1.1225553027,-0.0367799334\
O,-2.1984689969,-1.1176598988,0.0546115937\Si,-3.3238120863,0.1396038419,0.2937416892\
C,-4.9414615188,-0.7387914419,0.0622988859\N,-0.298337678,-2.077528878,-0.6610634538\
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C,-3.0330871779,1.4380679467,-1.0032917733\C,1.4117284756,-2.6462236584,-0.3379572643\
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Dipolar Intermediate

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C,-3.1621593505,3.4839981825,0.6433801526\C,-0.9513889486,0.344950799,-1.0113544273\
C,-0.1466966551,-0.6117939162,-0.2429864829\O,-0.6475927298,-1.796204026,-0.0112274312\
Si,-2.2570661815,-2.3939886455,0.0279216152\C,-2.0113668403,-4.086920078,0.7375150001\
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pop=nbo scrf=(solvent=dichloroethane)\\TS-C..C\\0,1\
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C,-0.7495044549,-1.1850713003,1.7765981119\C,1.8428519215,1.0099146284,3.9128994672\
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Product H

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scrf=(solvent=dichloroethane)\\Product H\\0,1\

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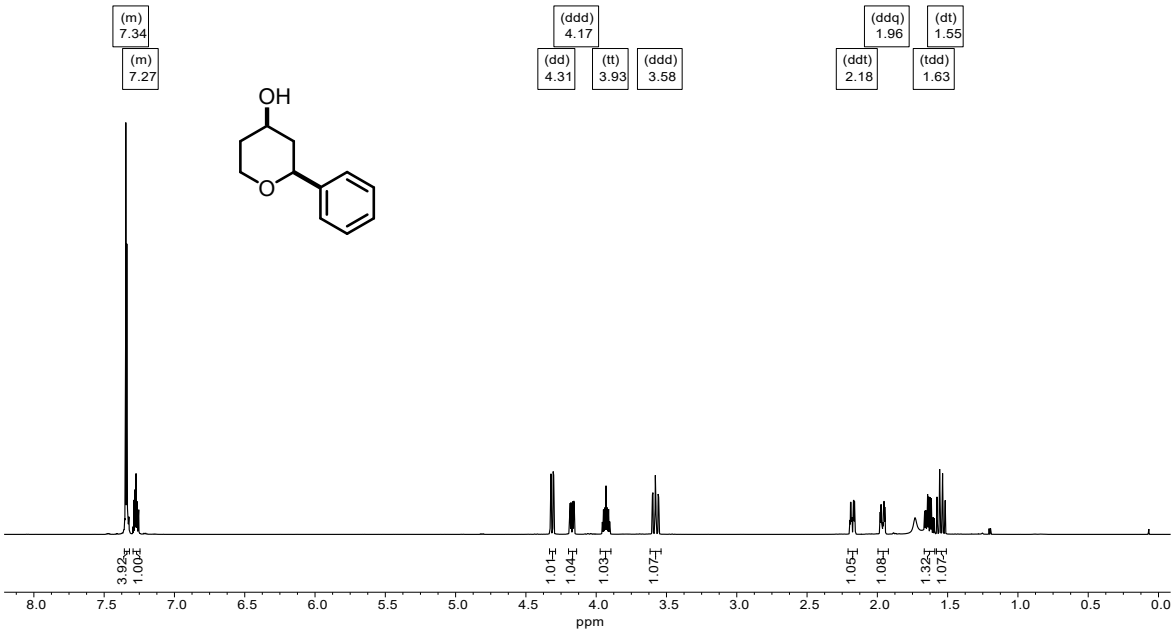
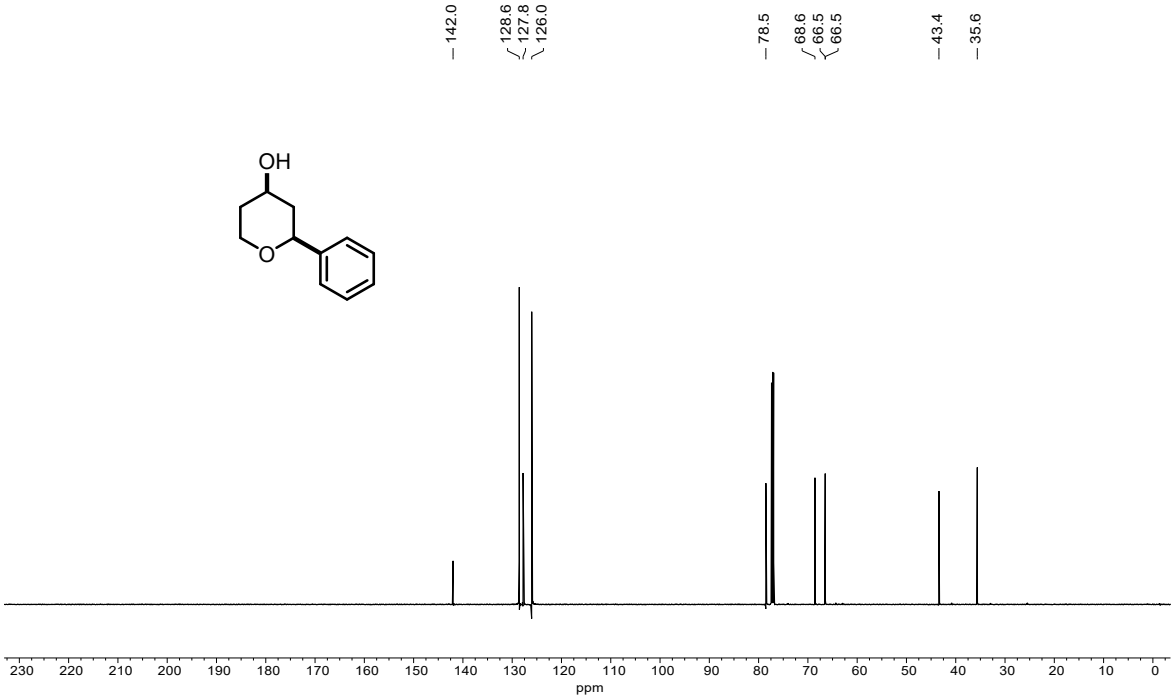
NMR Spectra



^{1}H NMR spectrum of *cis*-2-Phenyltetrahydro-2H-pyran-4-ol in $CDCl_3$.



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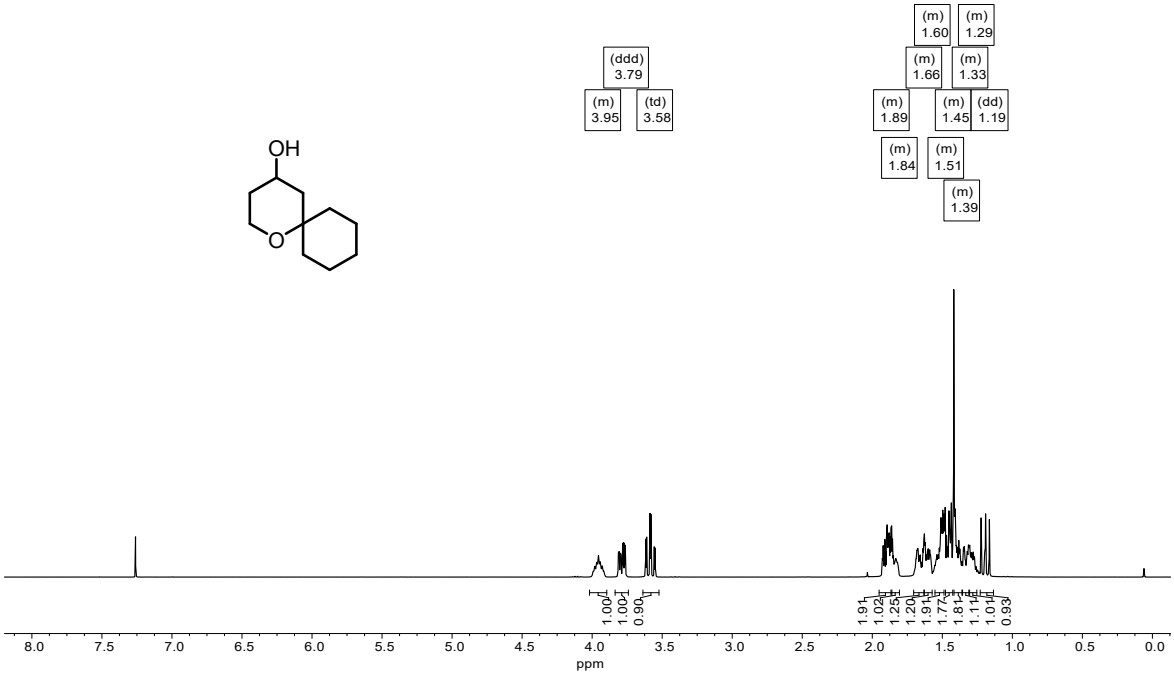
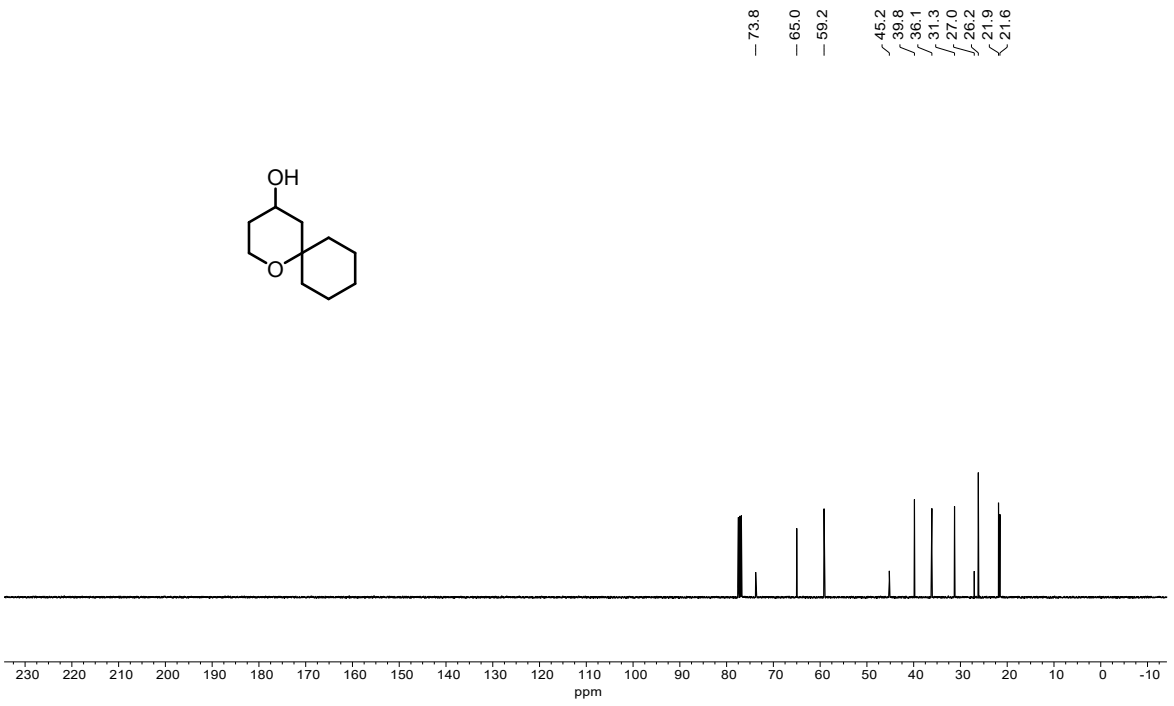


^{1}H NMR spectrum of (*RS*)-1-Oxaspiro[5.5]undecan-4-ol in $CDCl_3$.



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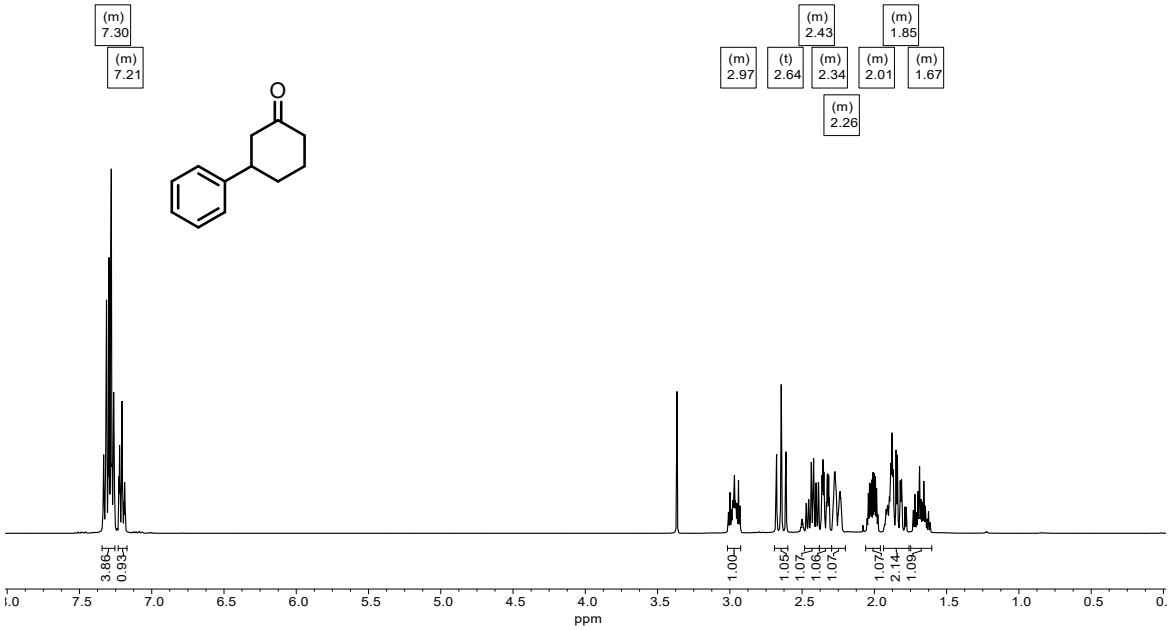
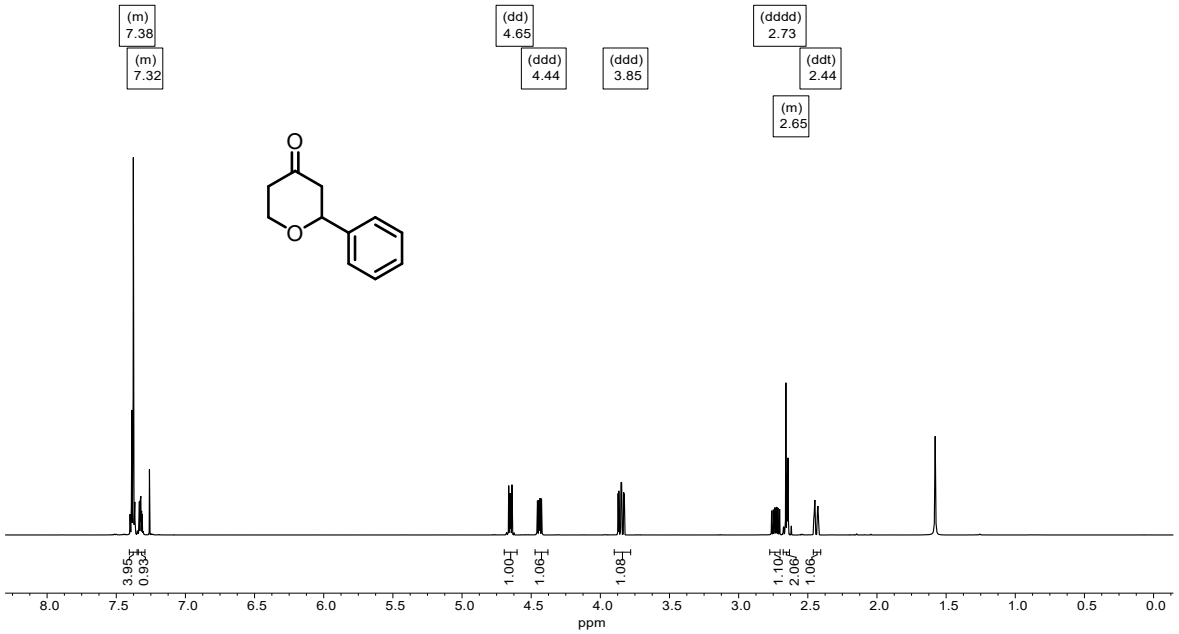


^{1}H NMR spectrum of **3** in $CDCl_3$.

^{13}C NMR spectrum of **3** in $CDCl_3$.



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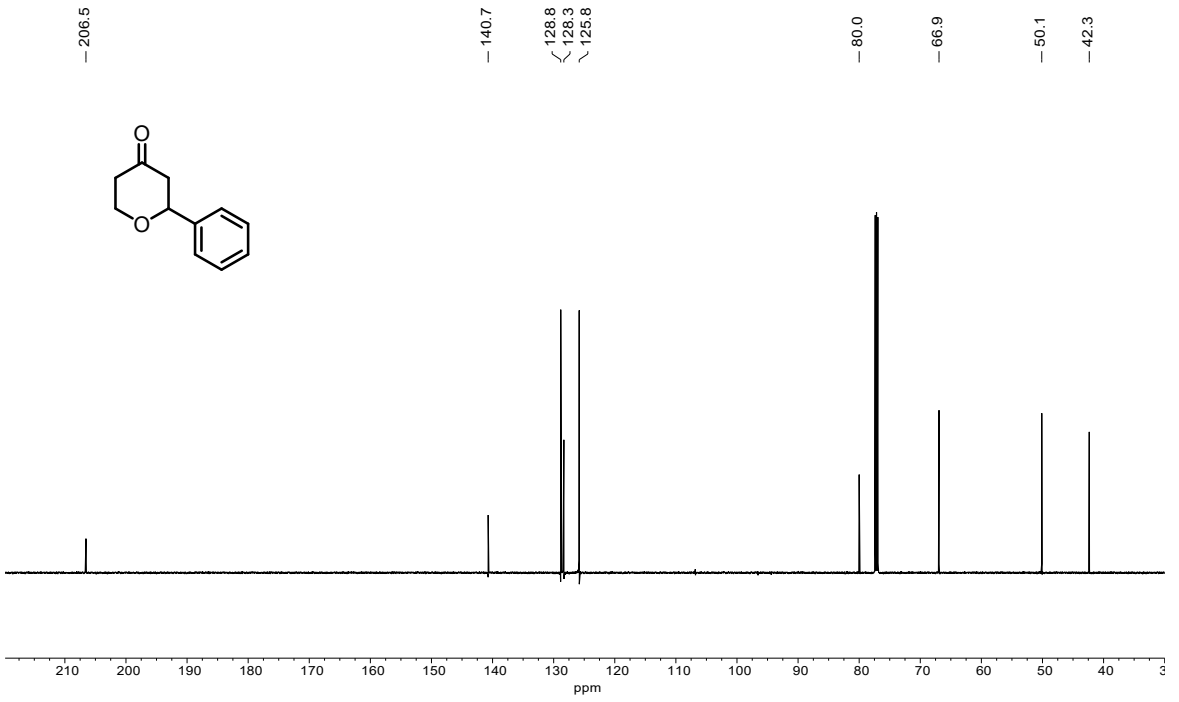

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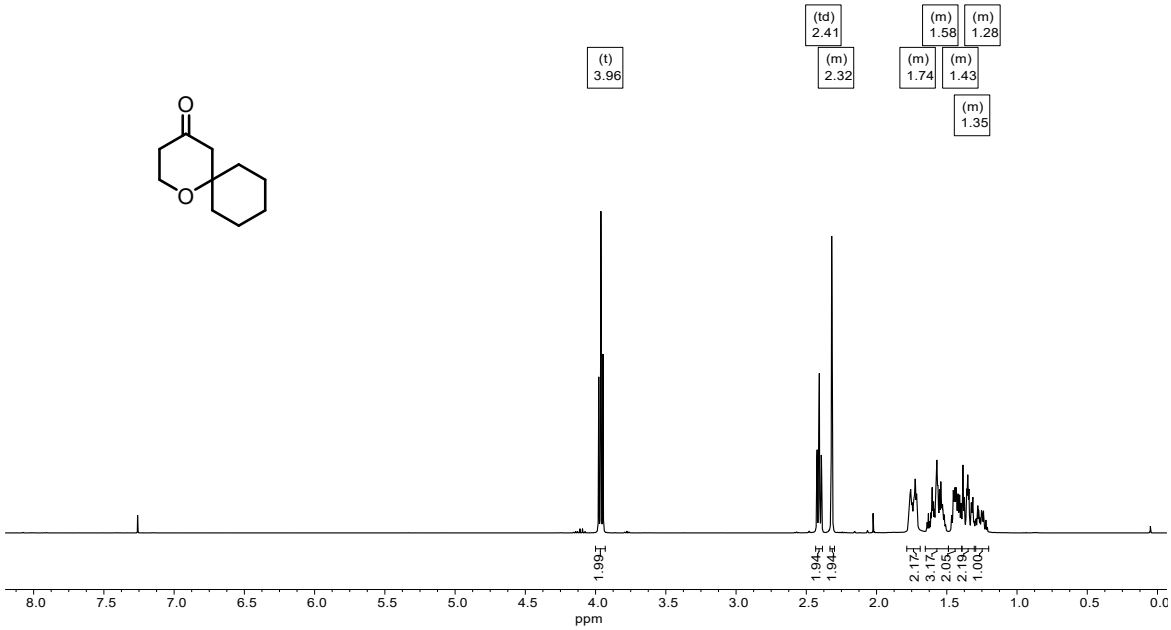

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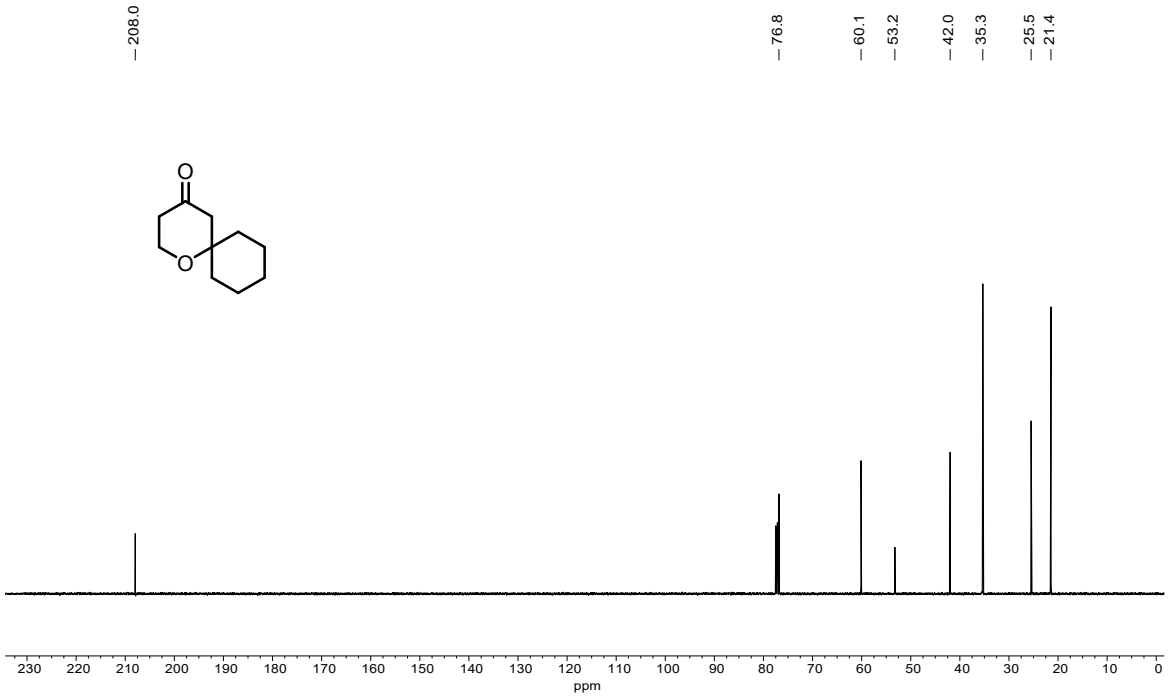

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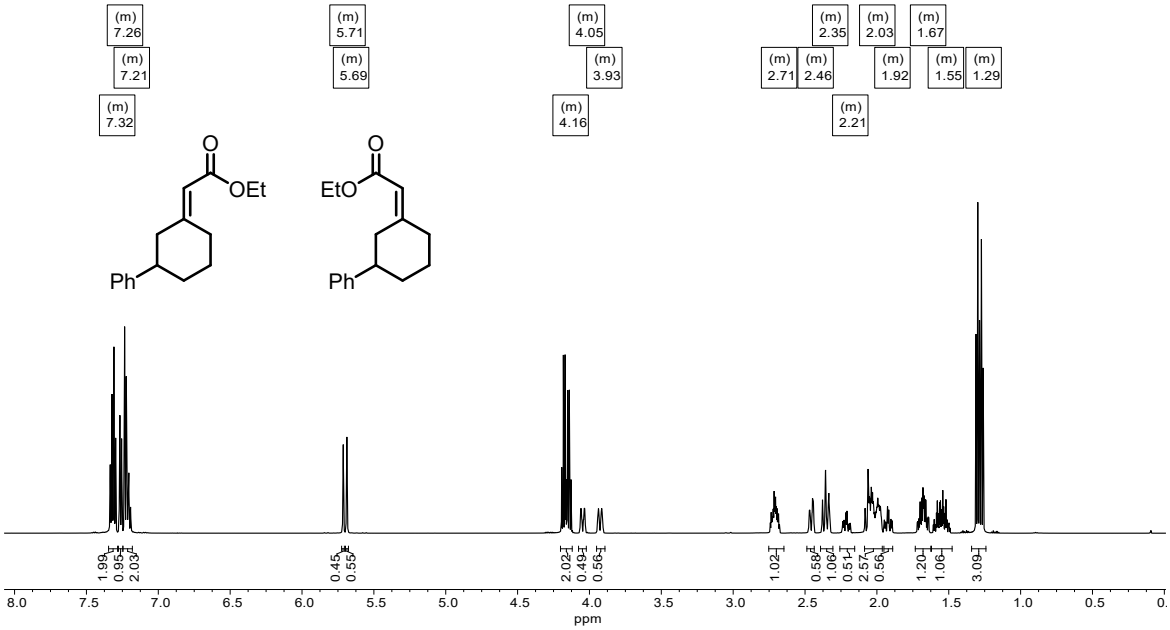
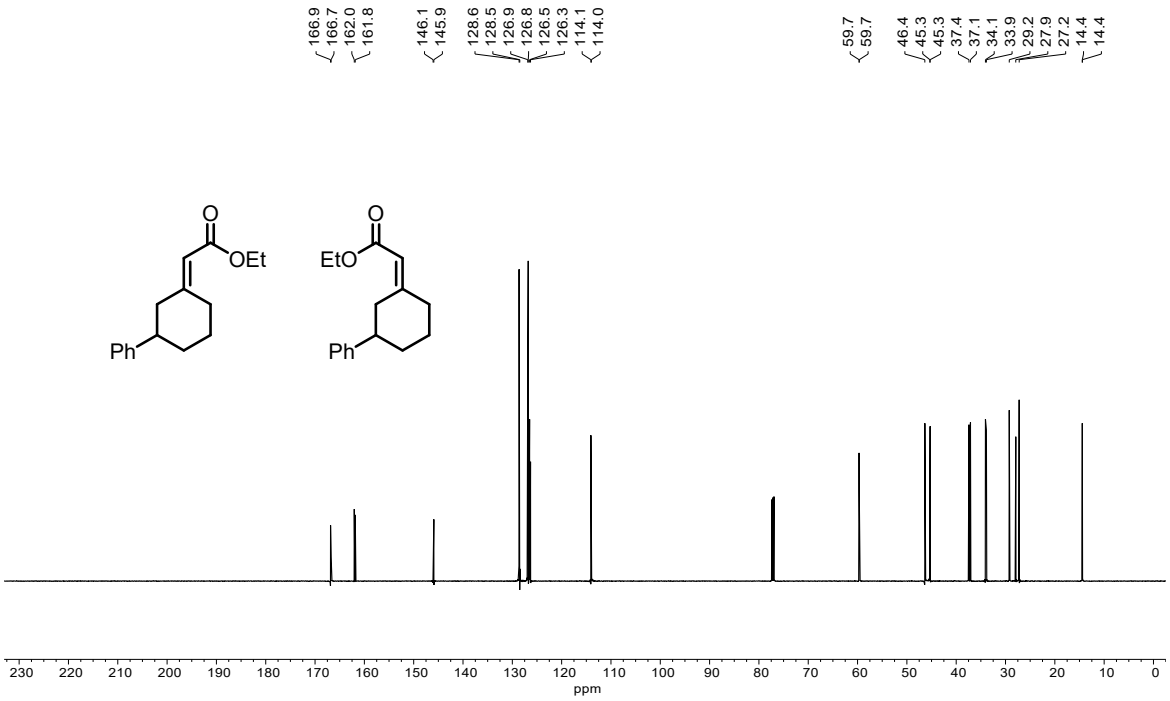
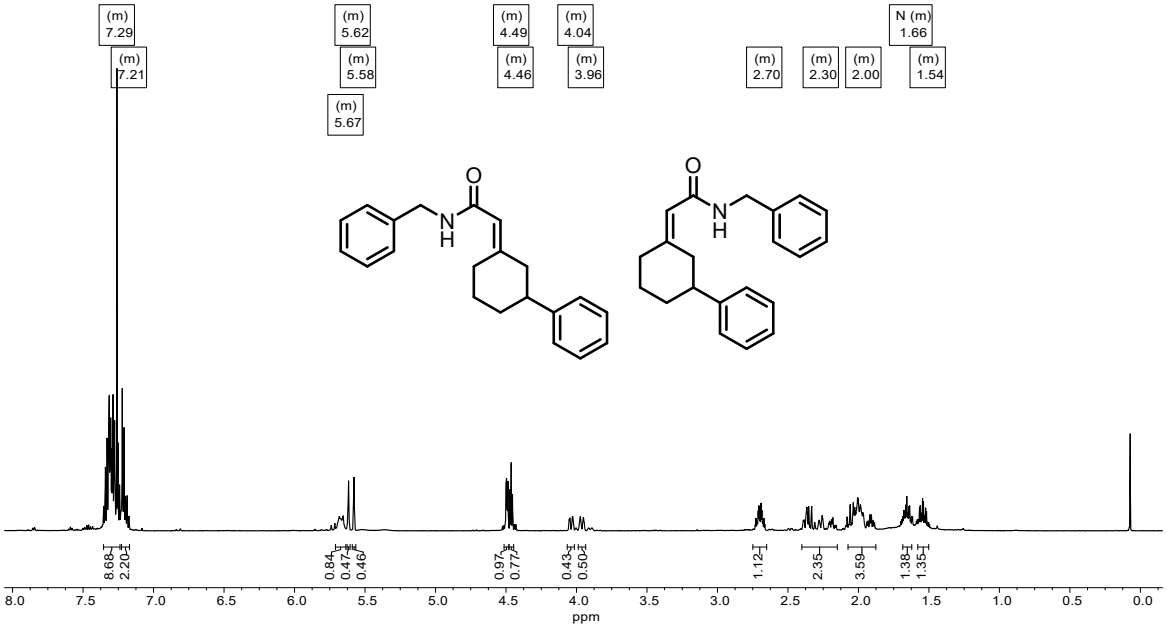


^{1}H NMR spectrum of (*E*)-**4** and (*Z*)-**4** in $CDCl_3$.



^{13}C NMR spectrum of (*E*)-**4** and (*Z*)-**4** in $CDCl_3$.



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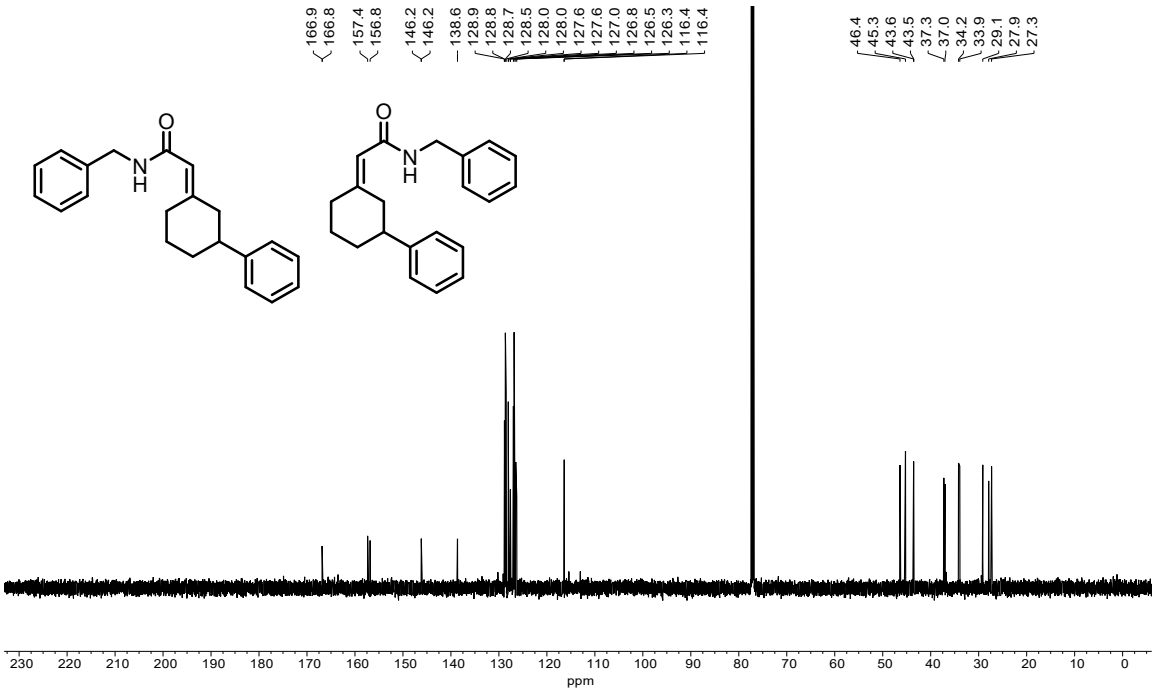

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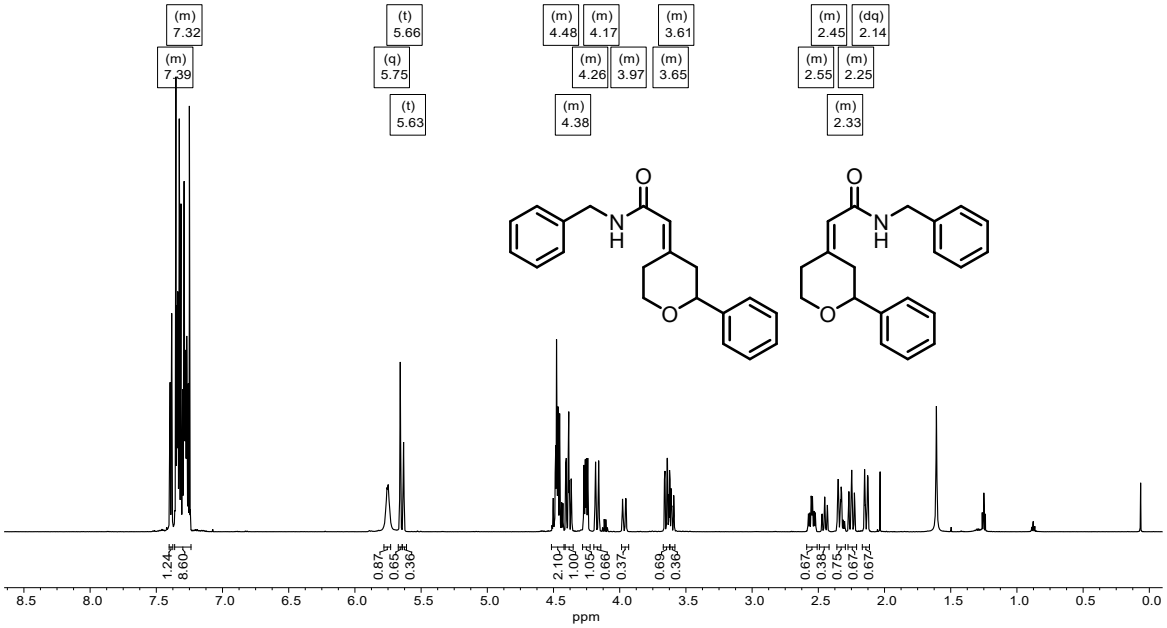
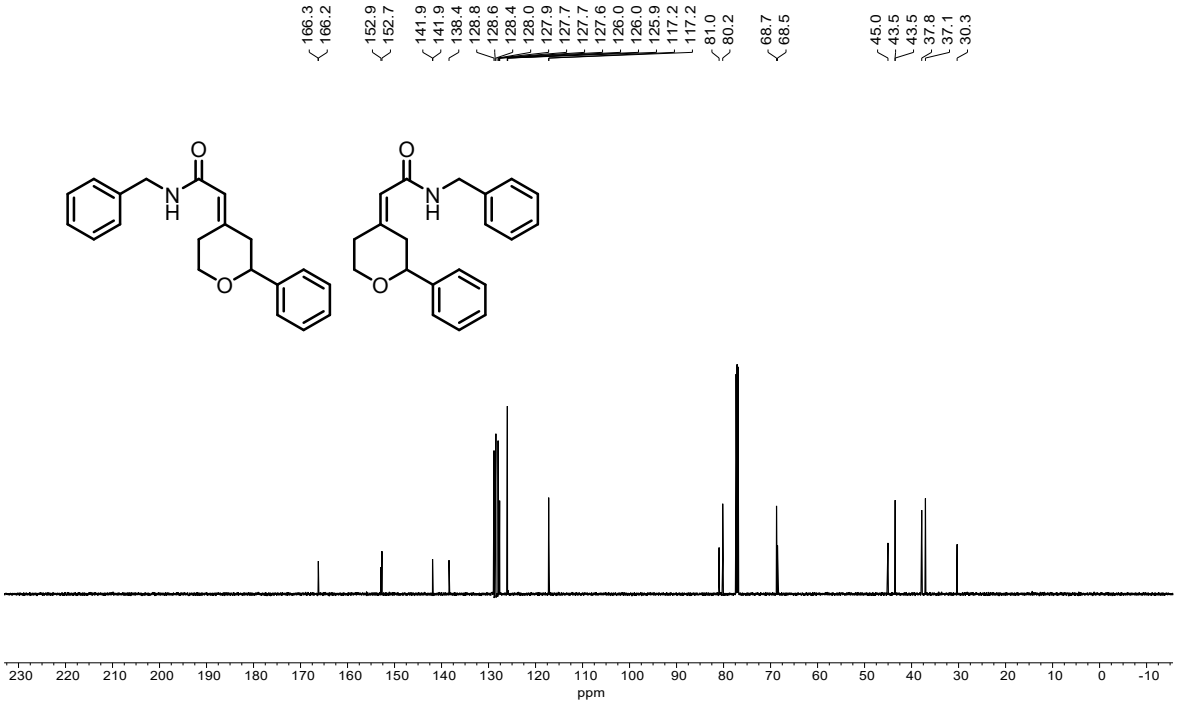


^{1}H NMR spectrum of (*E*)-**13** and (*Z*)-**13** in $CDCl_3$.



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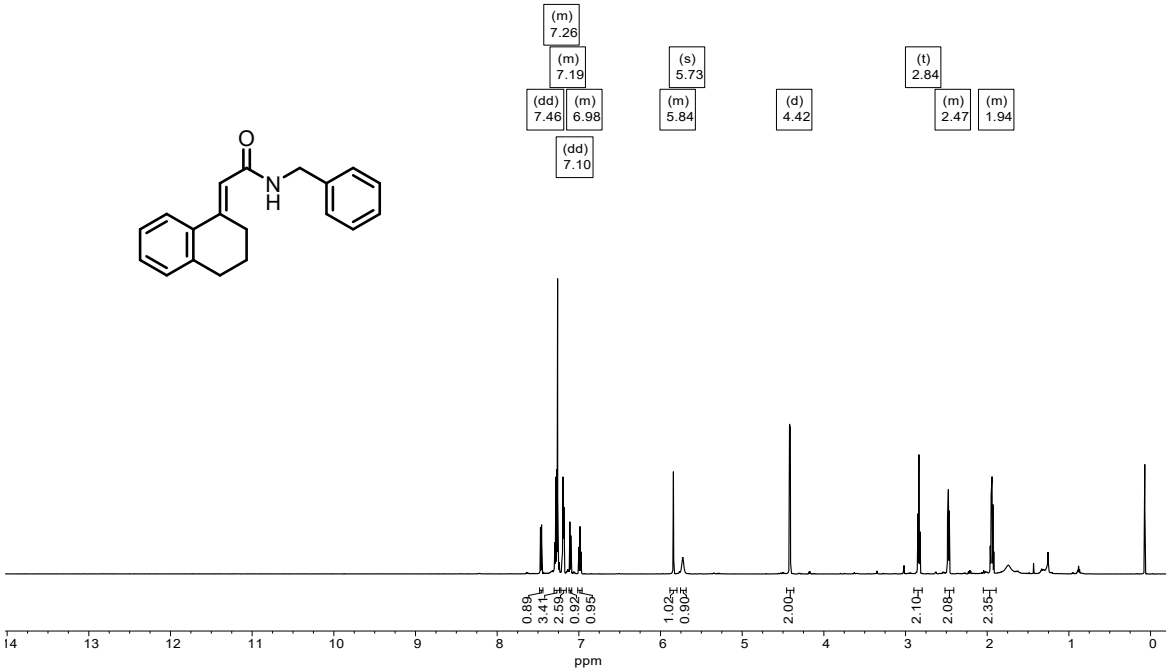

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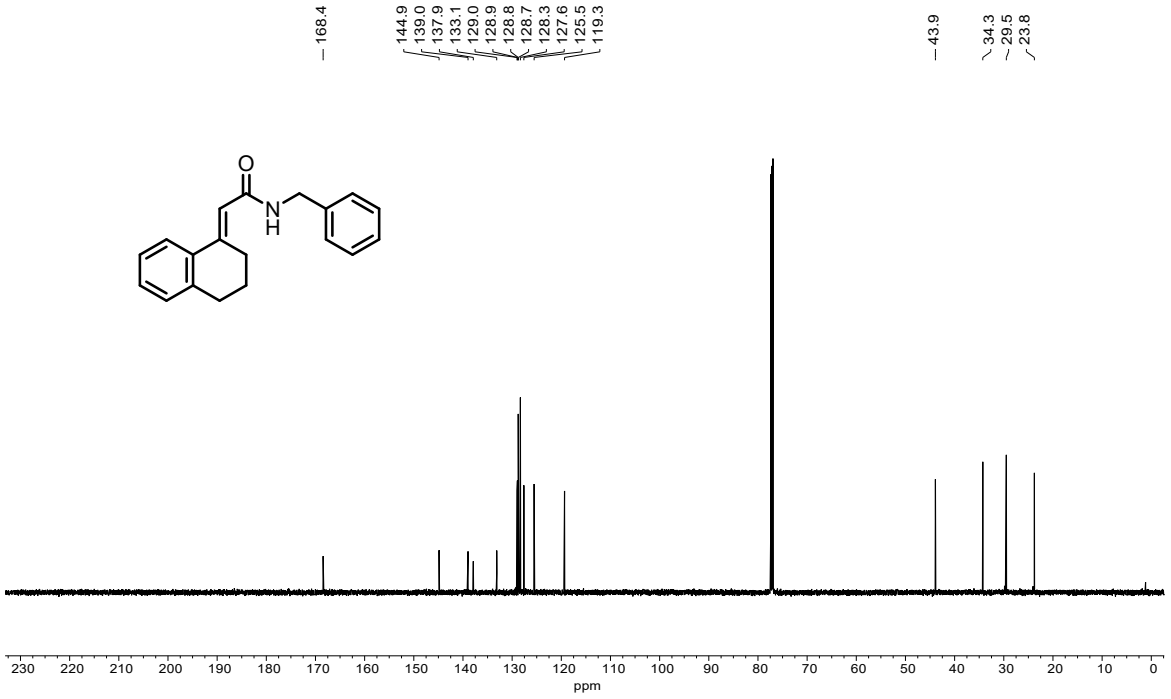

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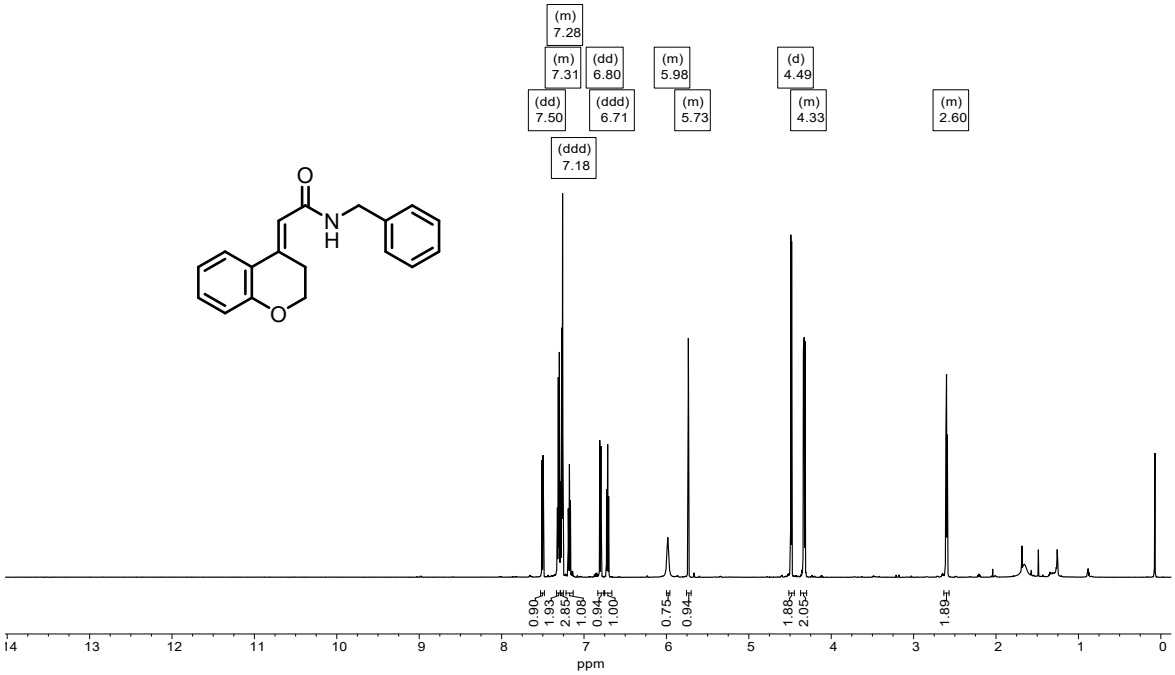

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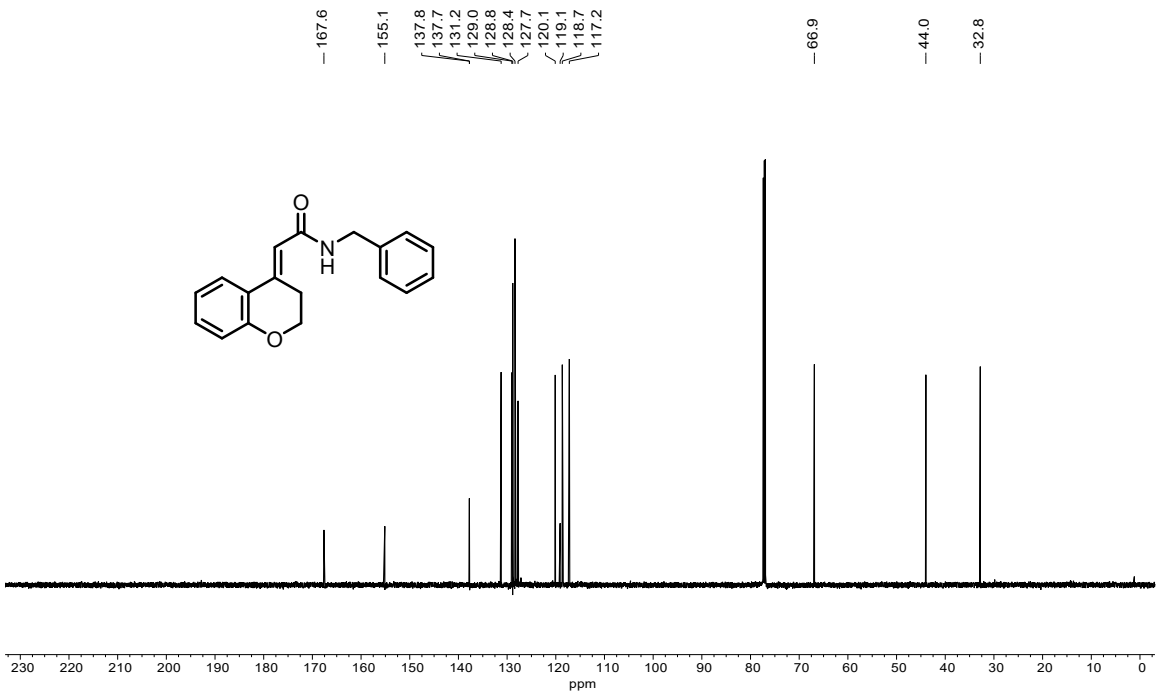

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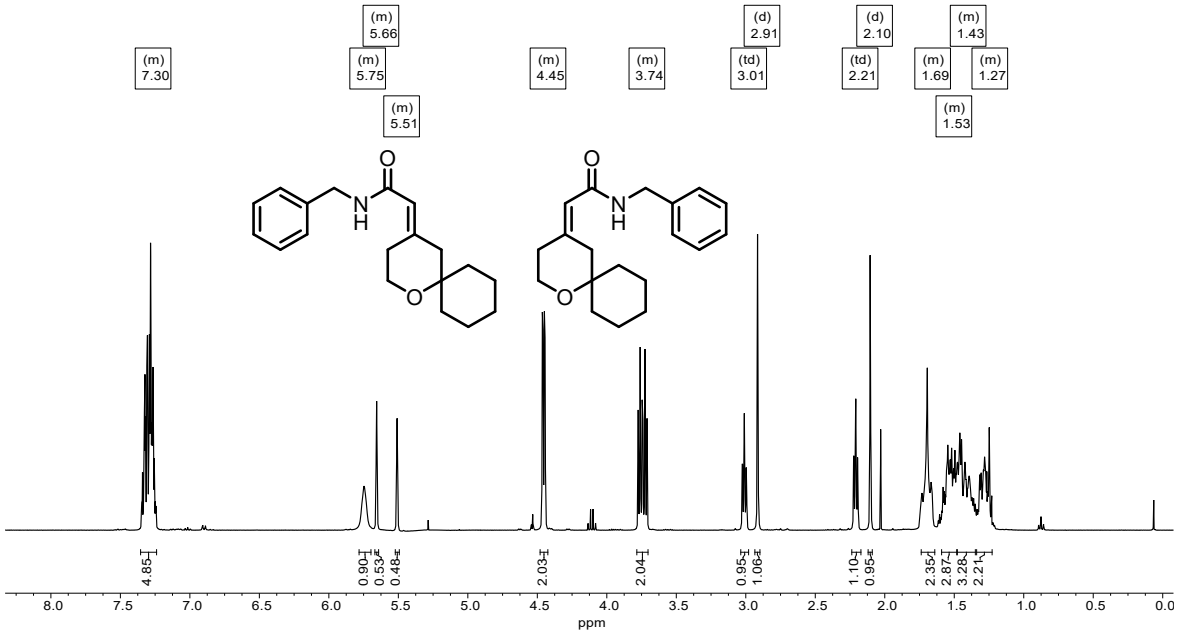

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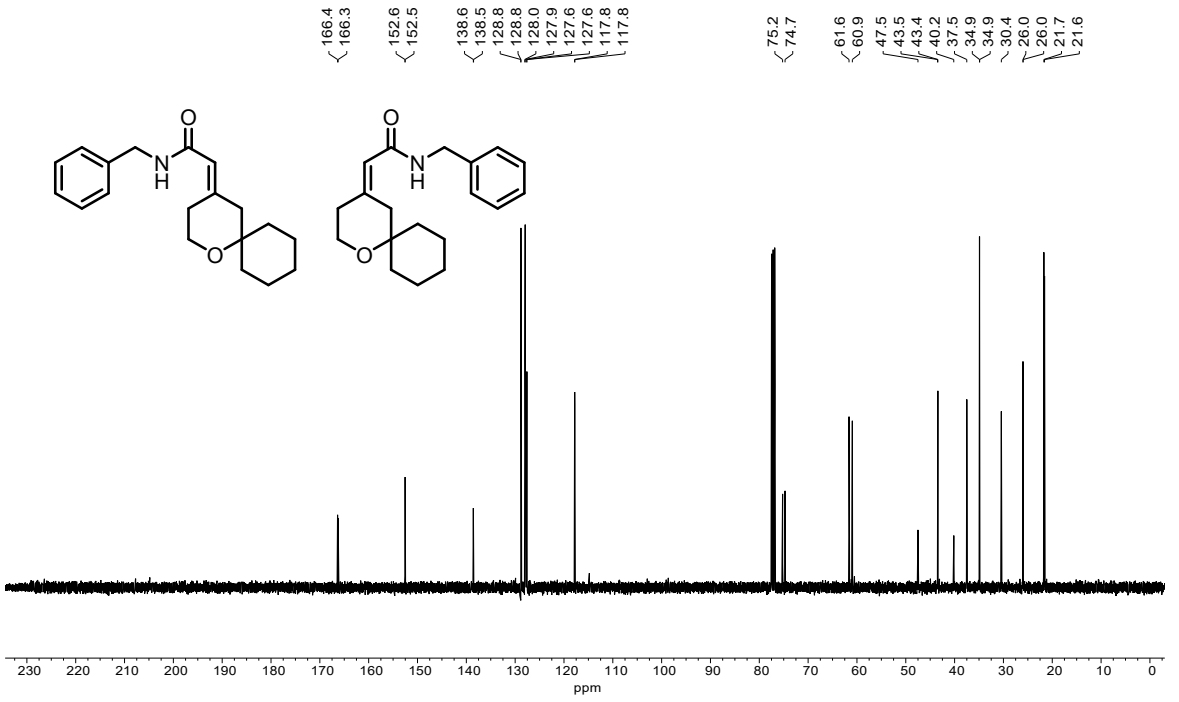

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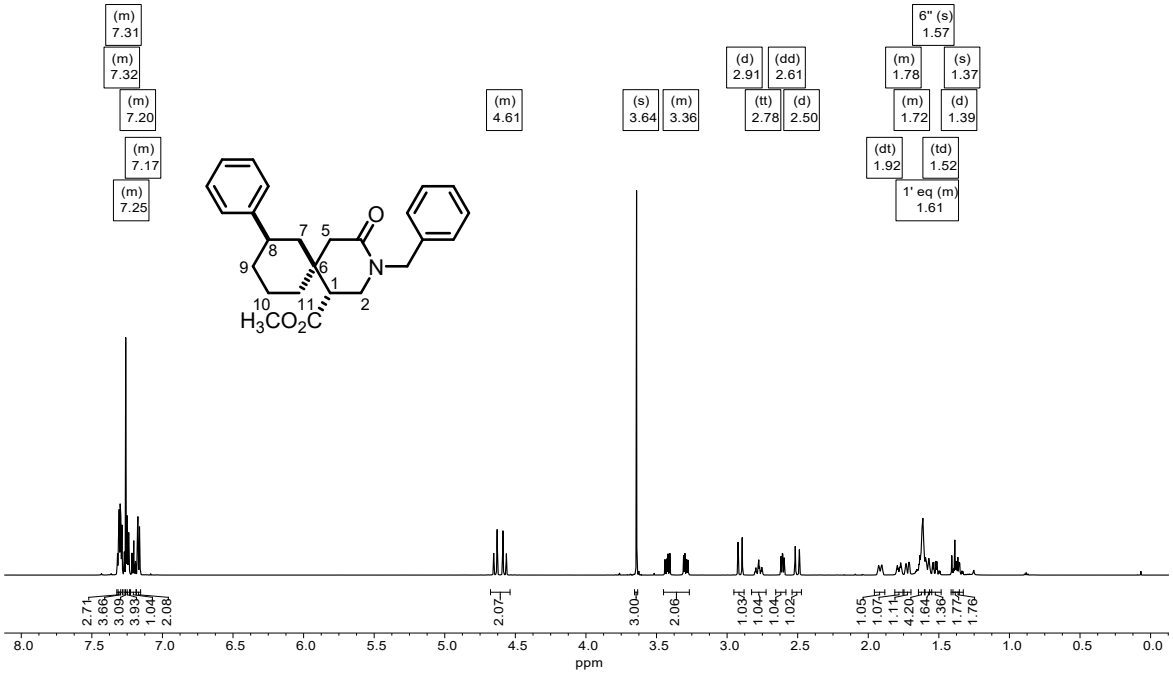
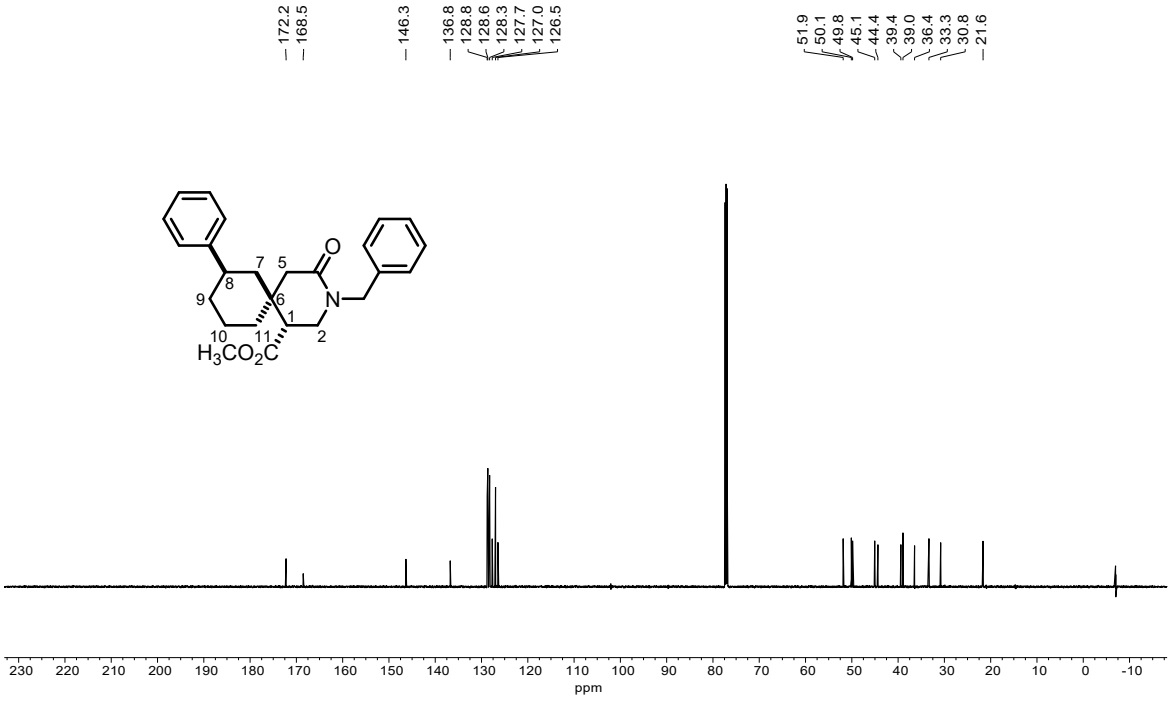


^{1}H NMR spectrum of **8a** in $CDCl_3$.



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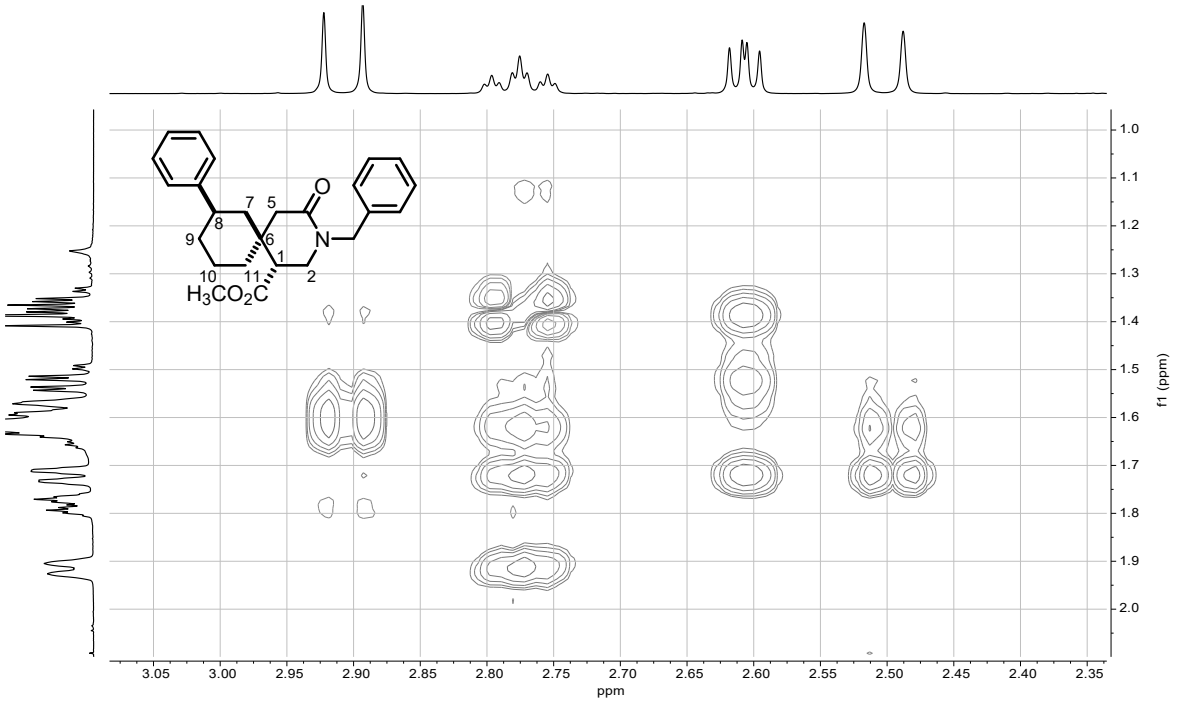
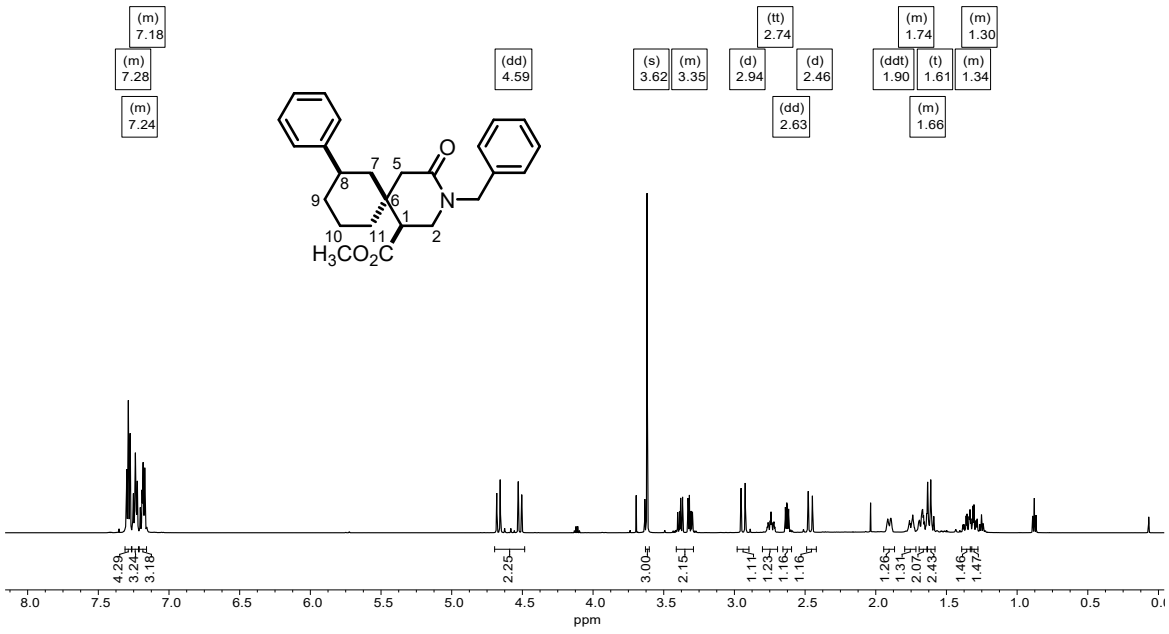


NOESY spectrum of **8a** in $CDCl_3$.



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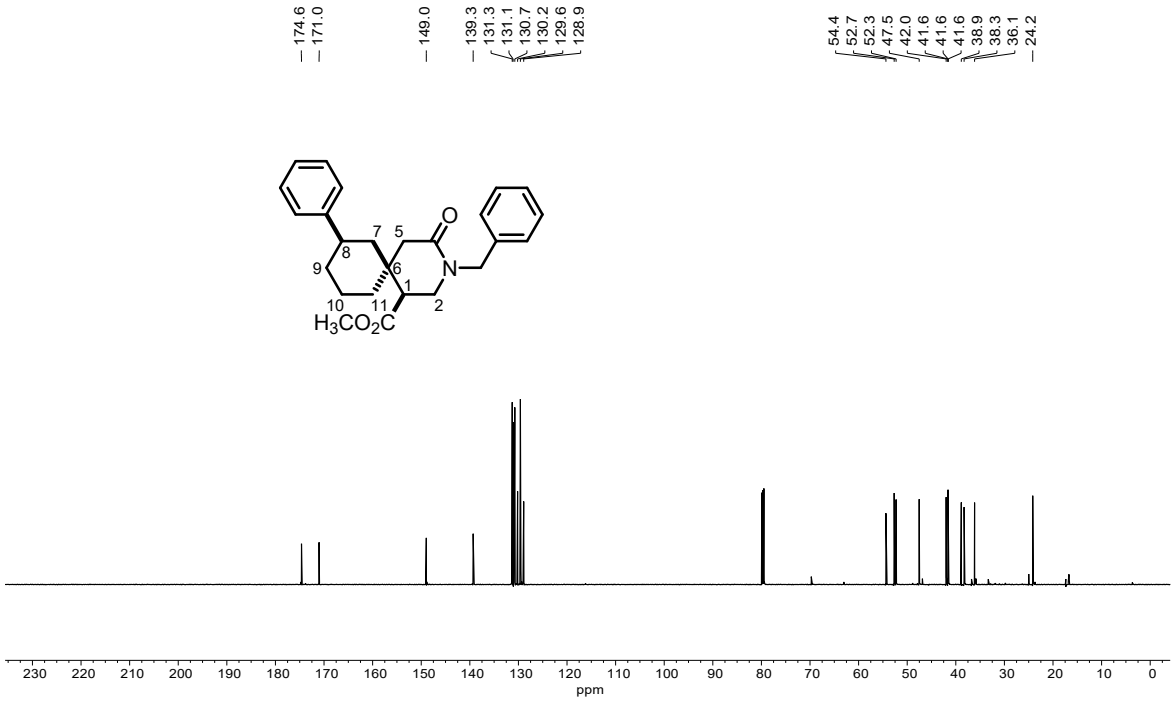

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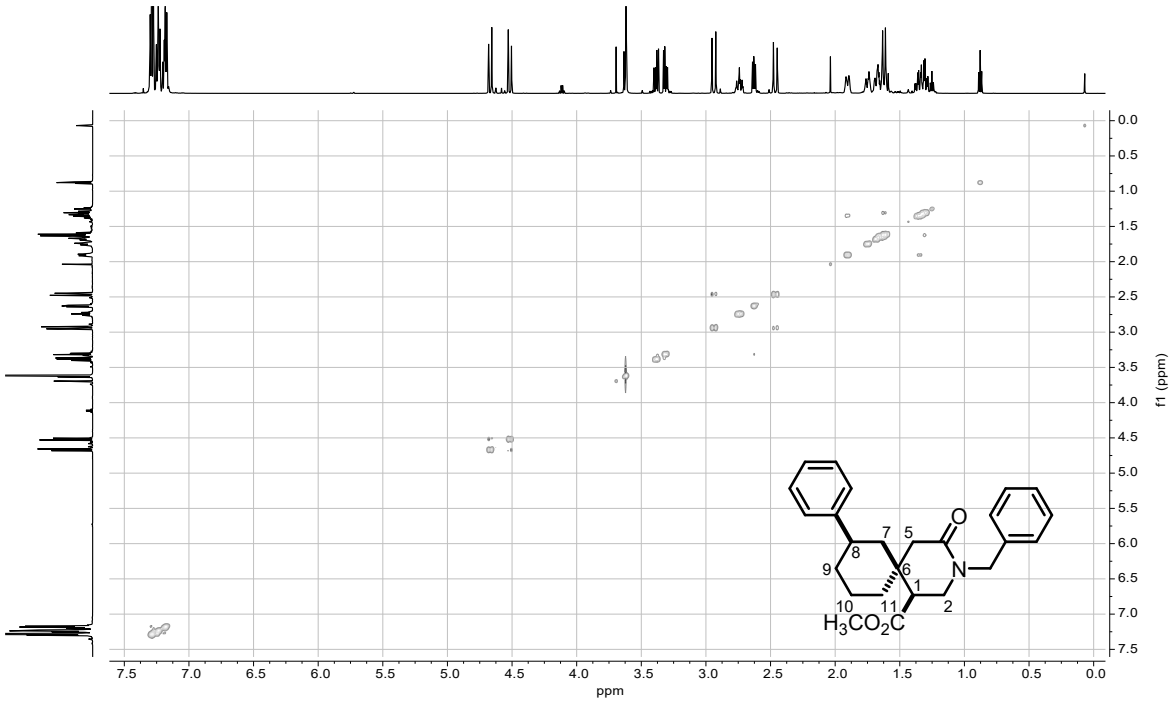

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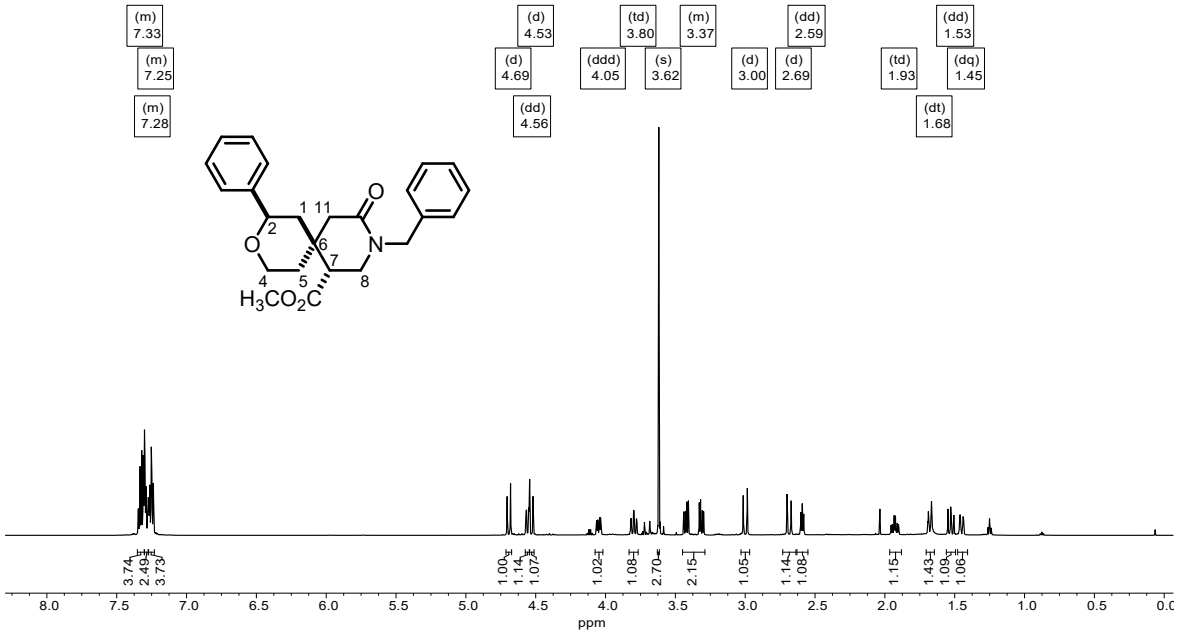

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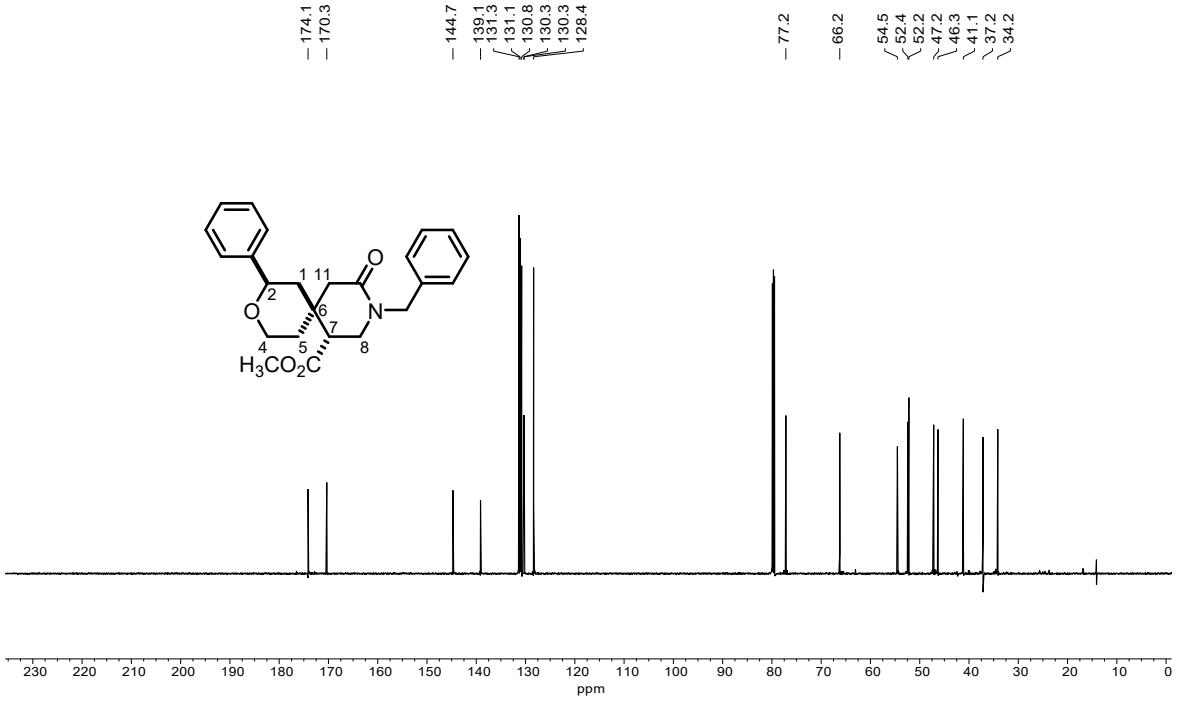

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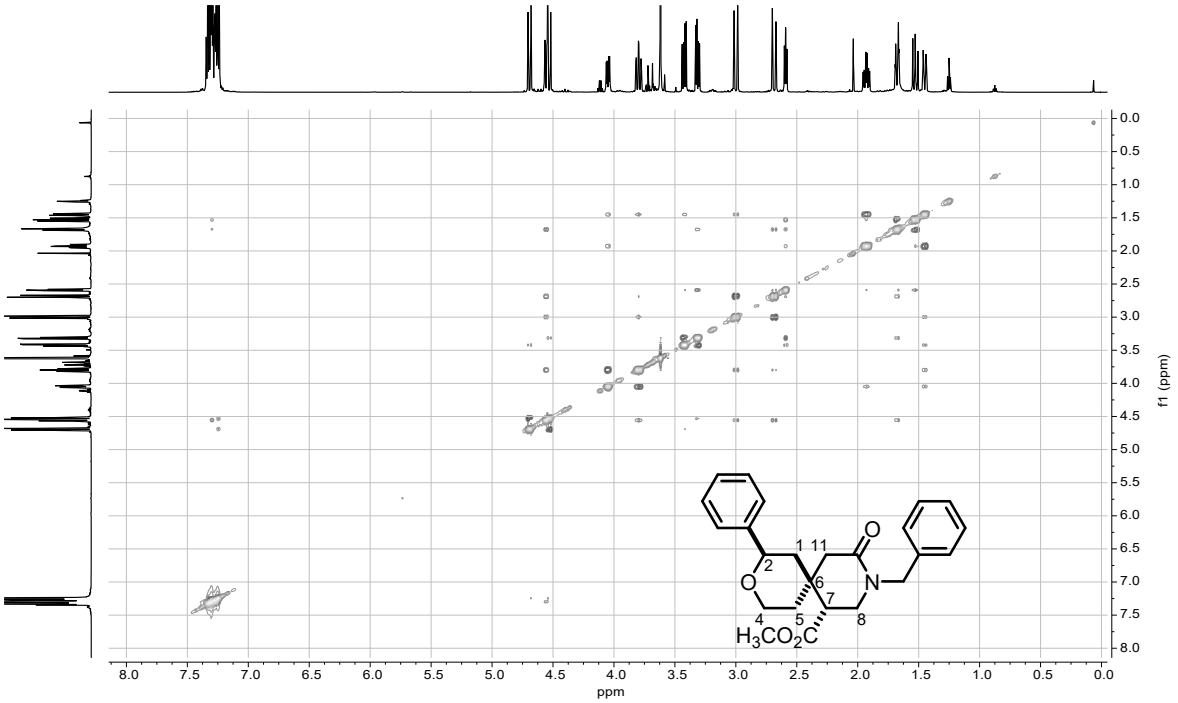
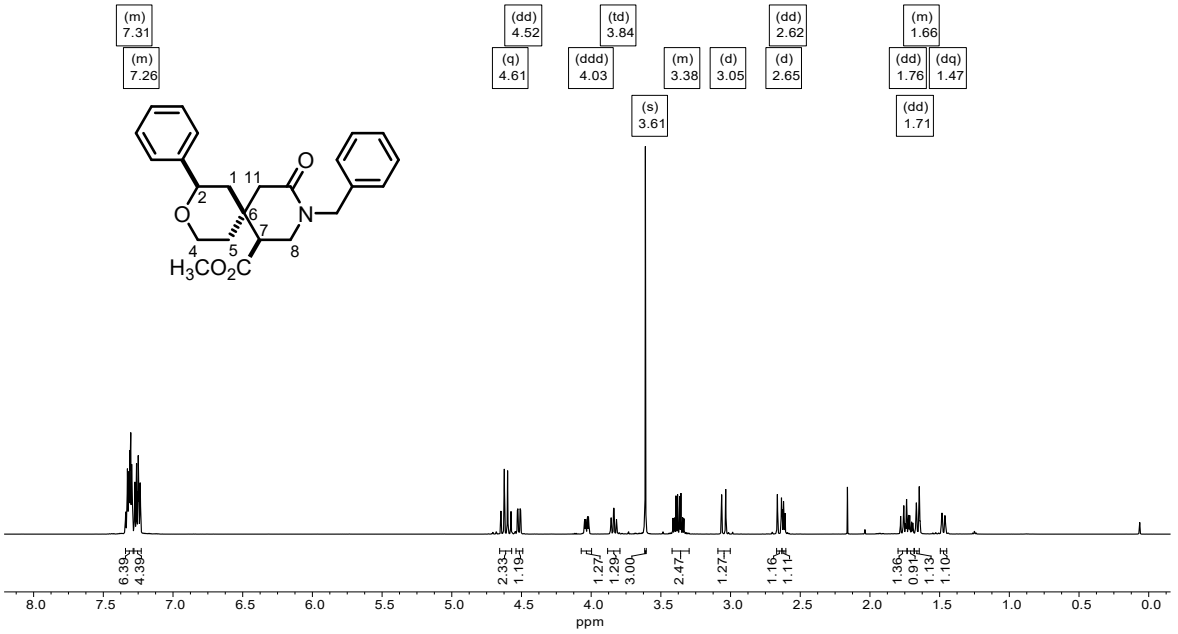


NOESY spectrum of **17a** in $CDCl_3$.



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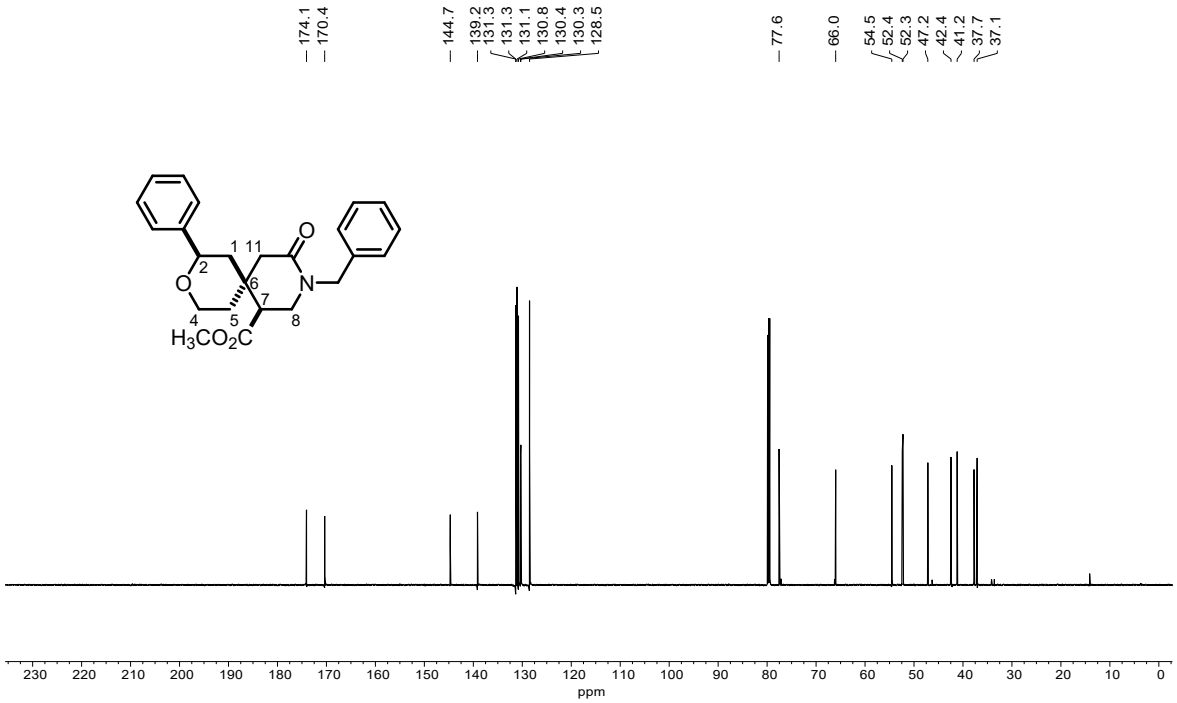

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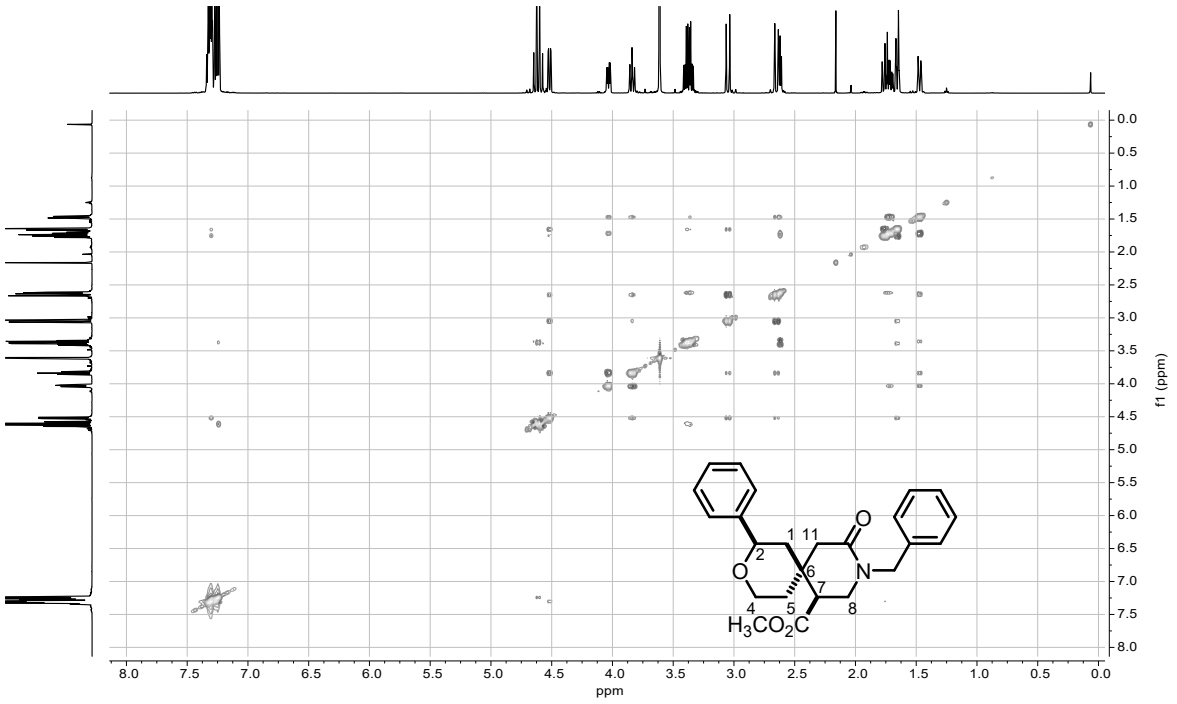

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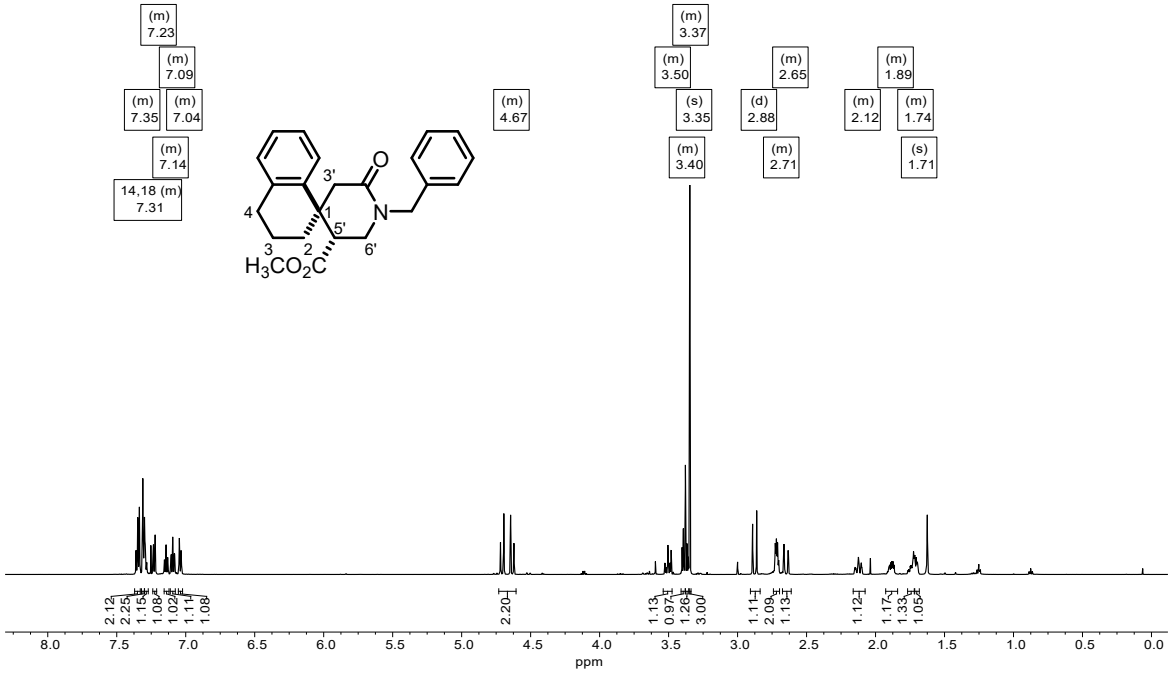

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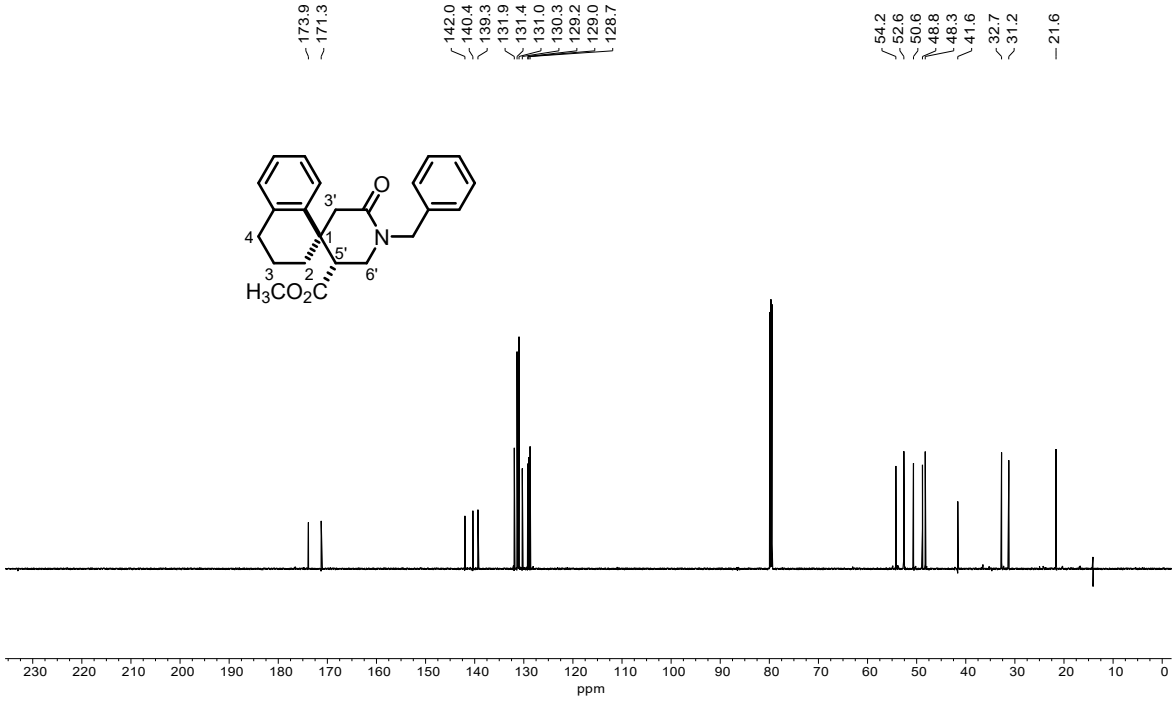

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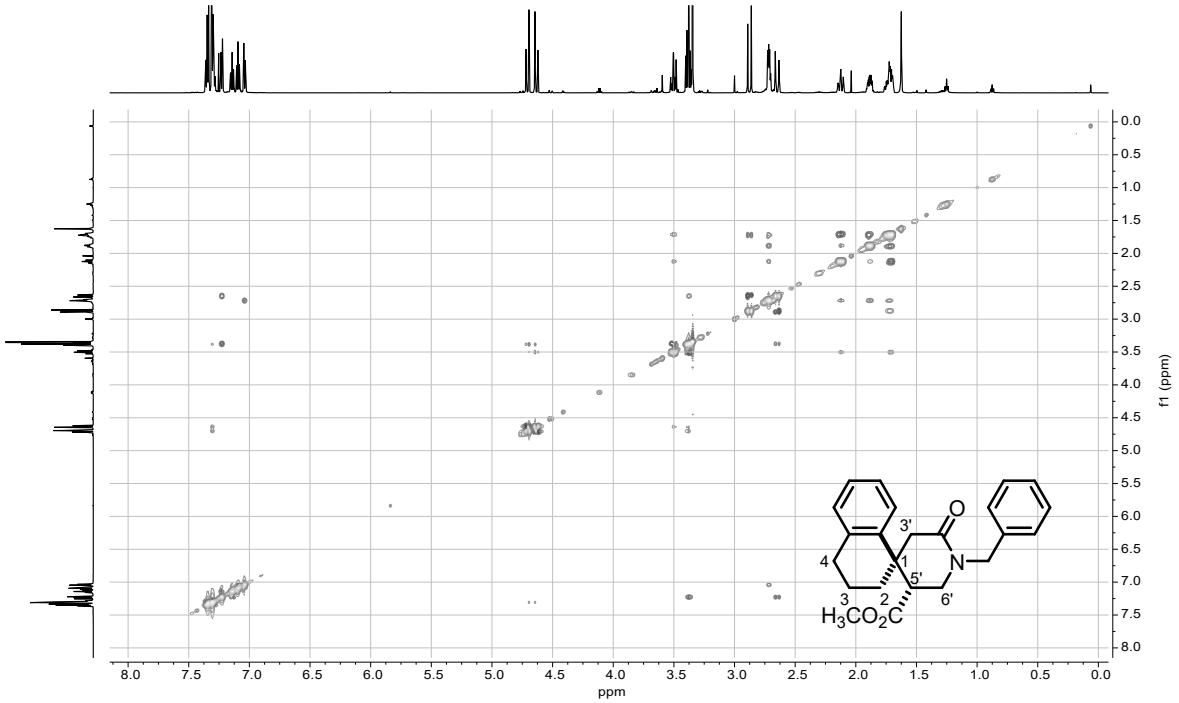

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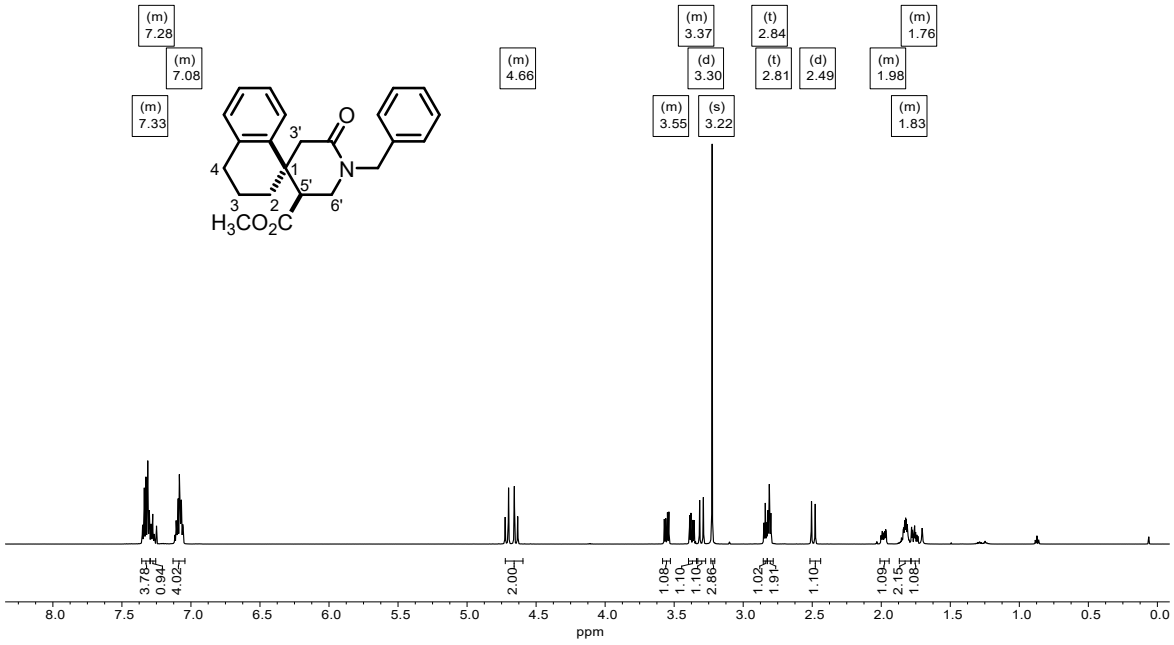

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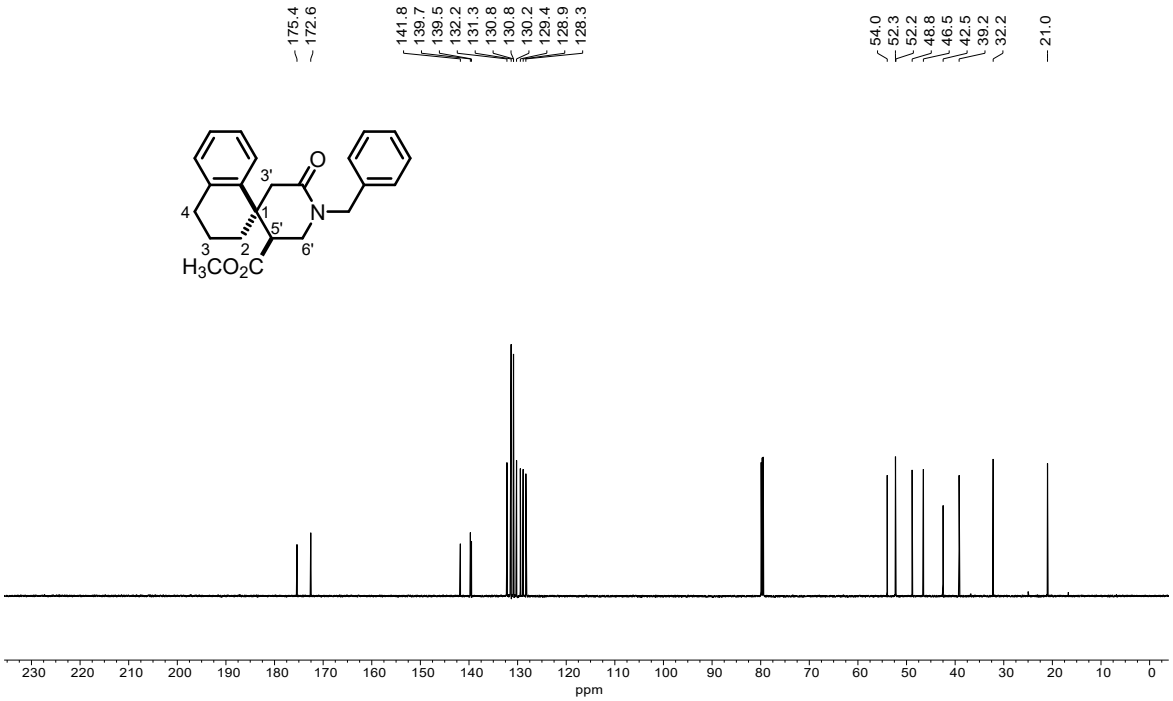

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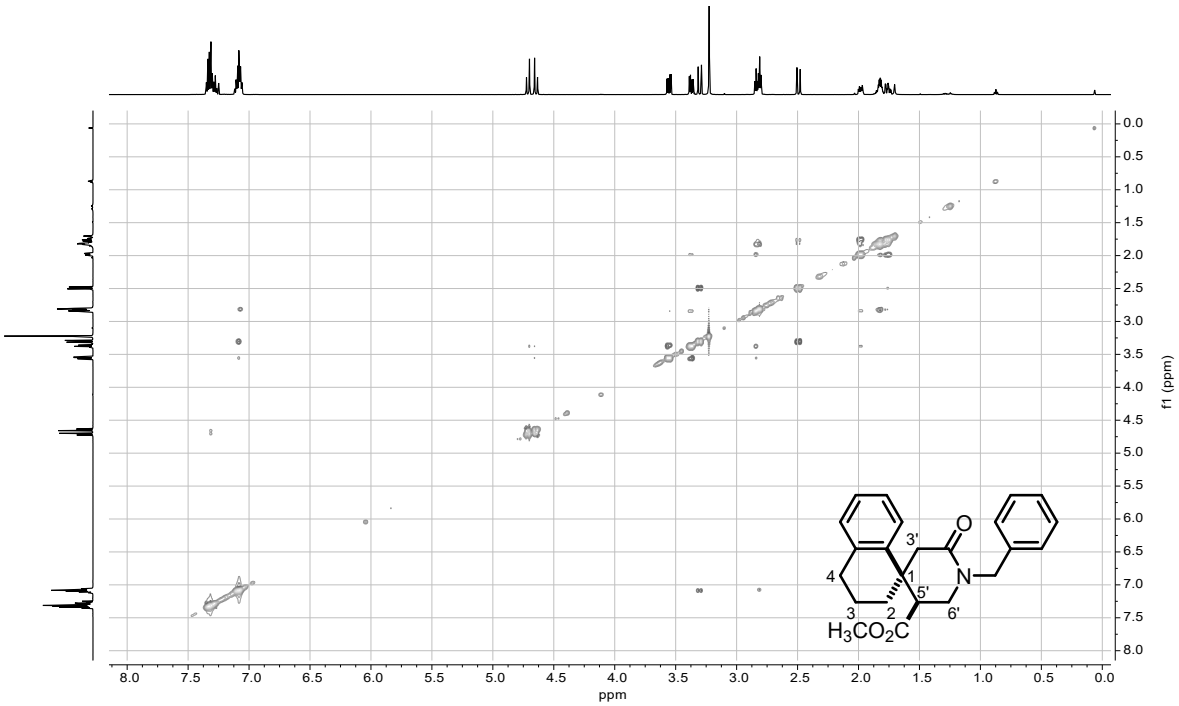

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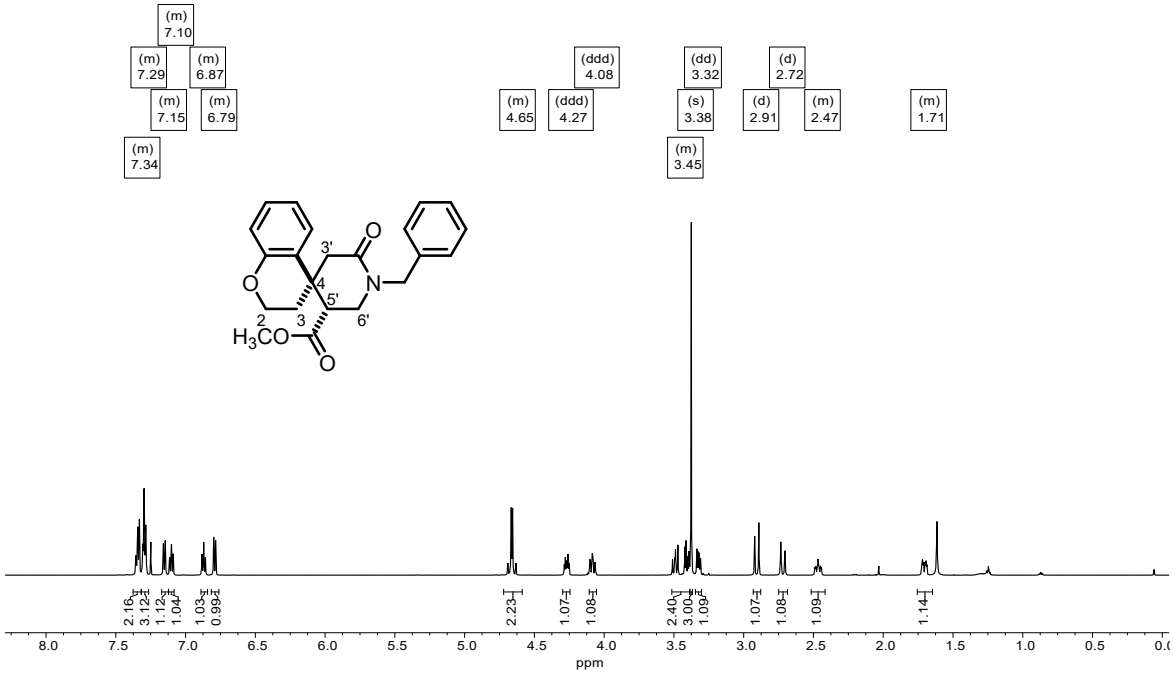

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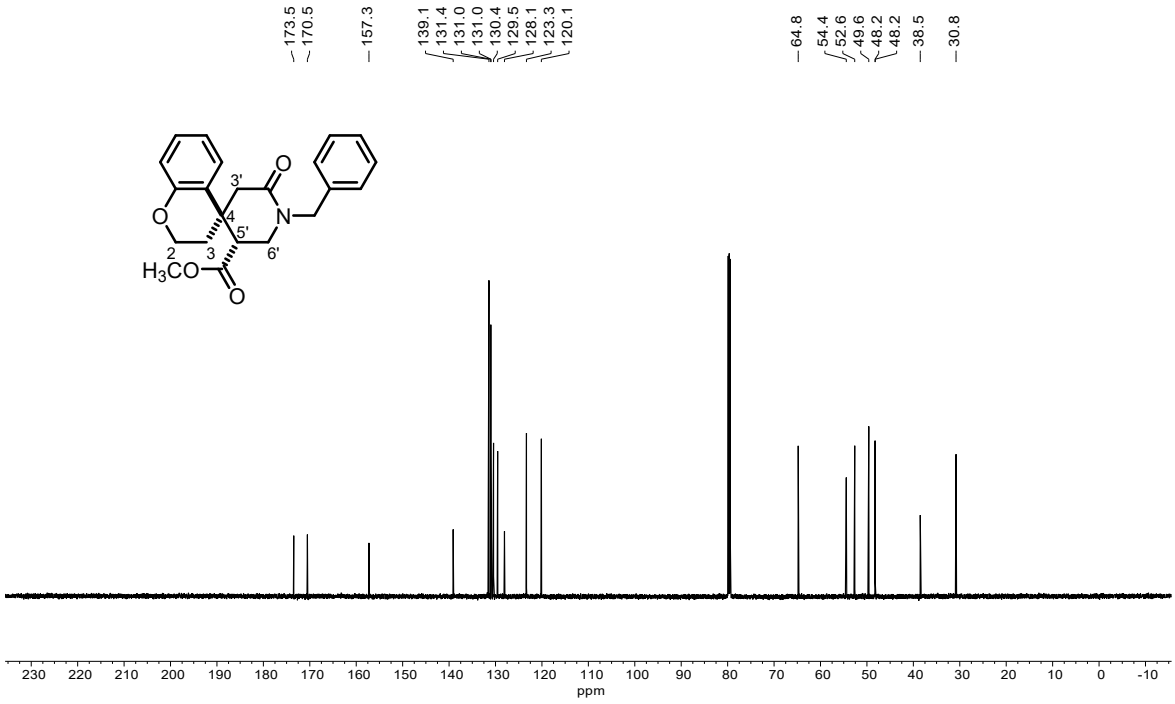

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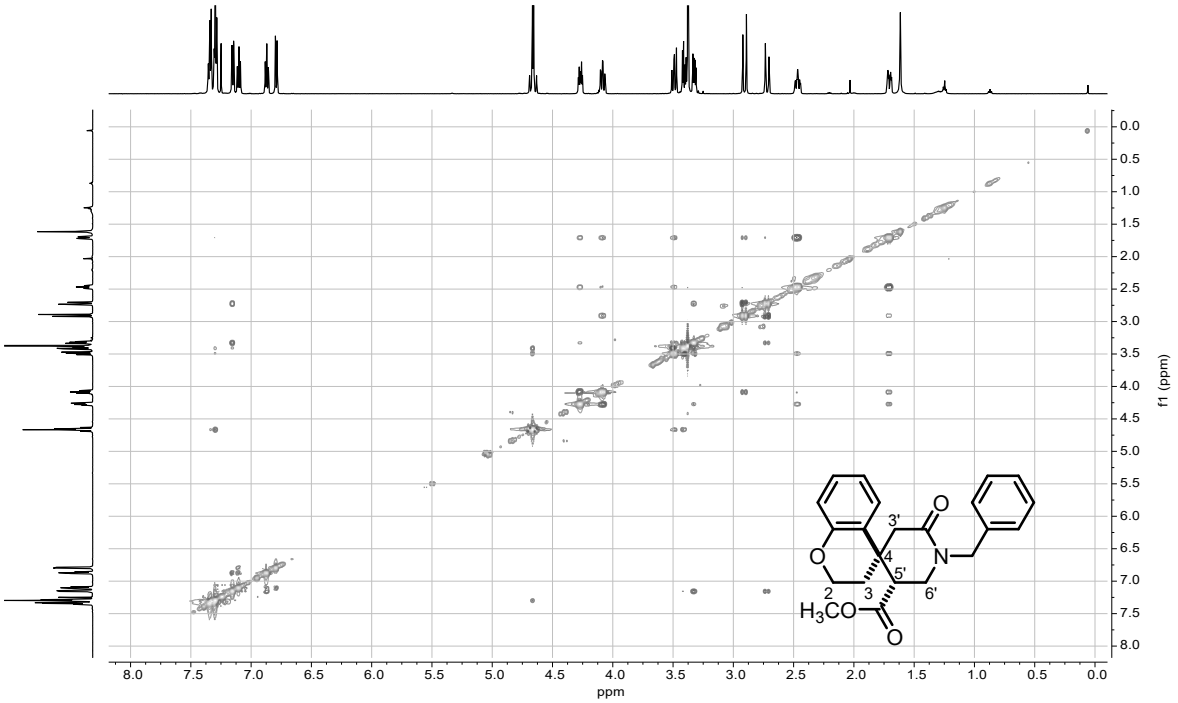

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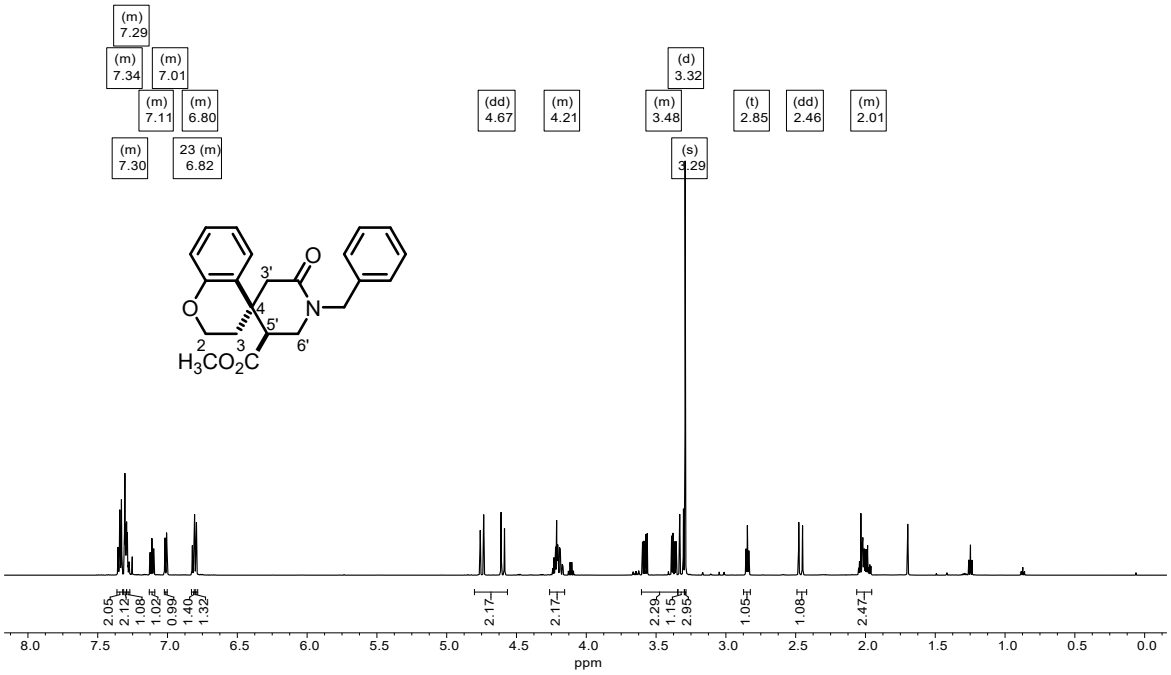

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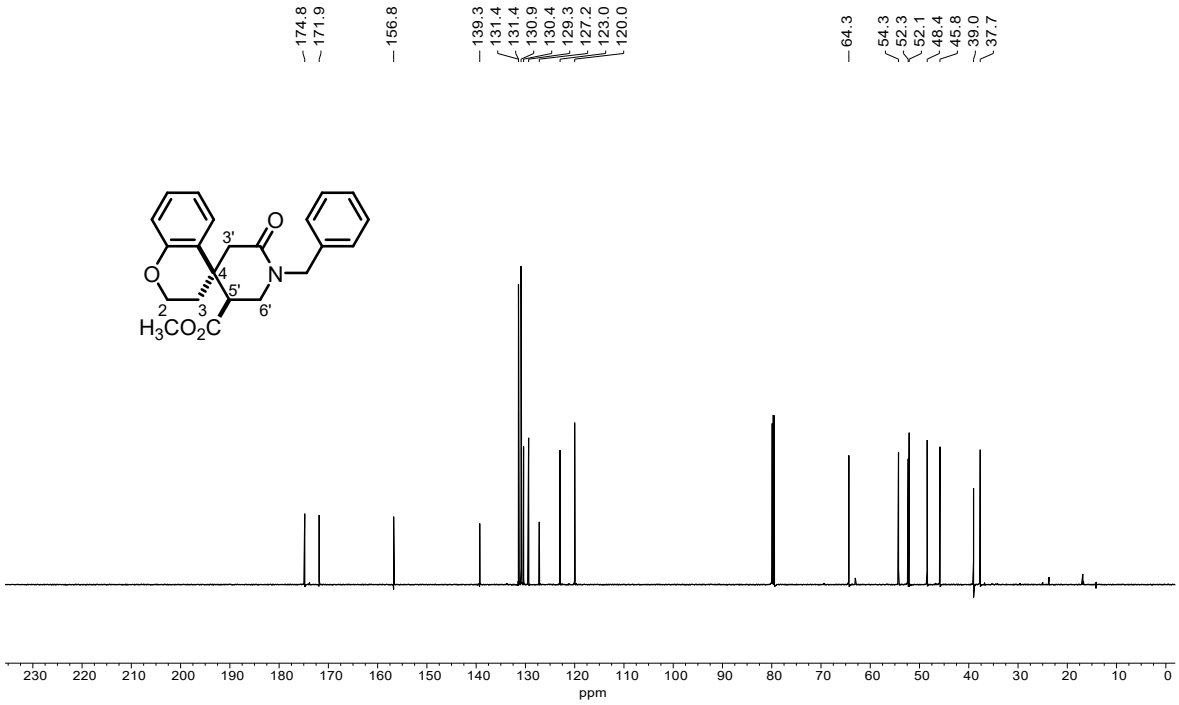

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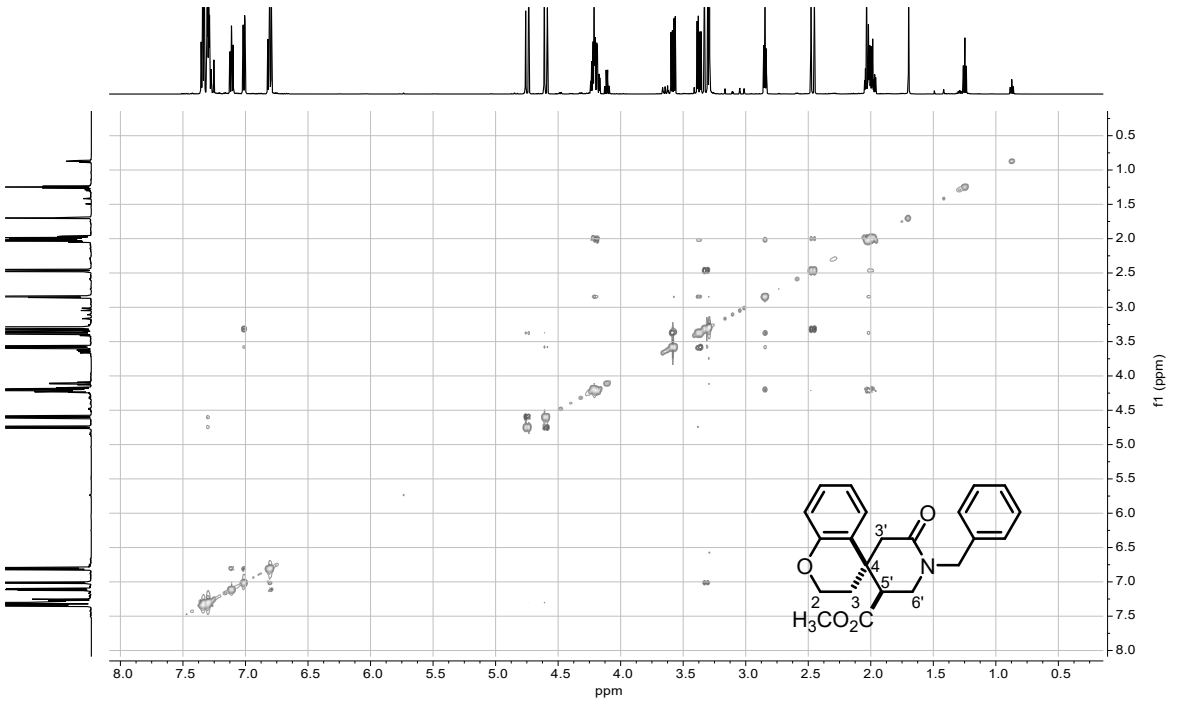

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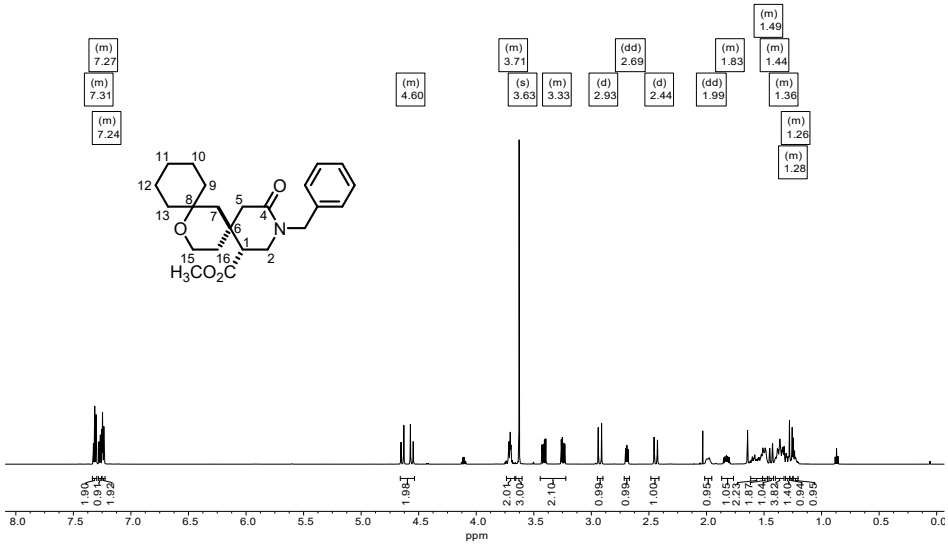

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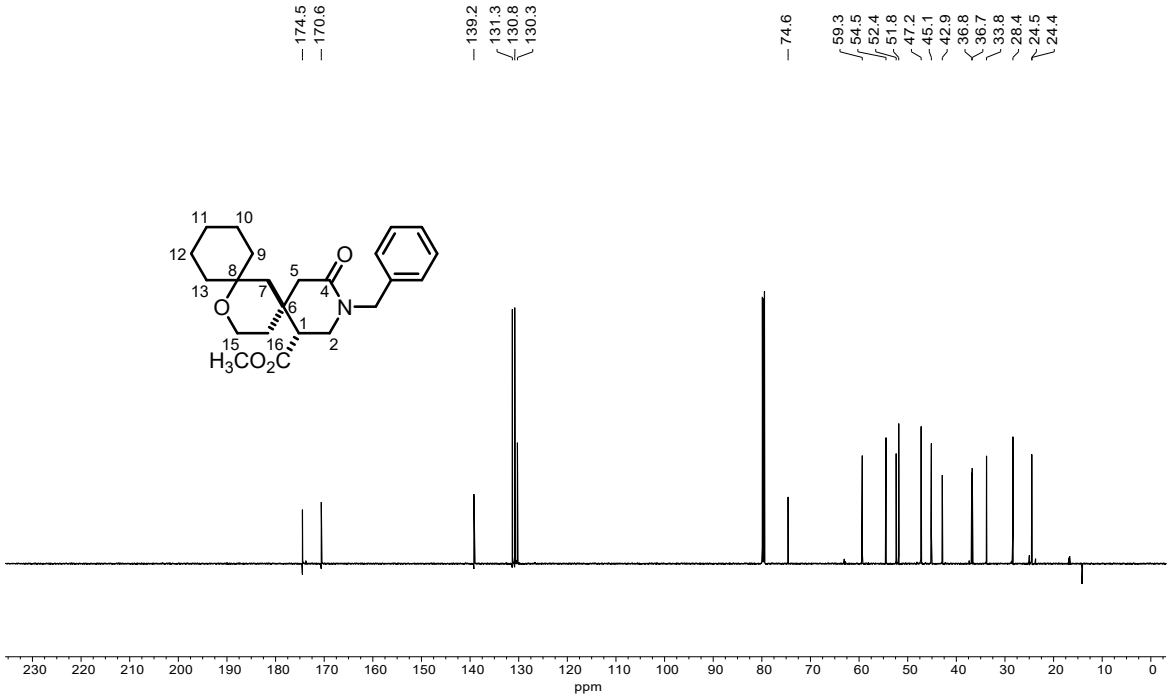

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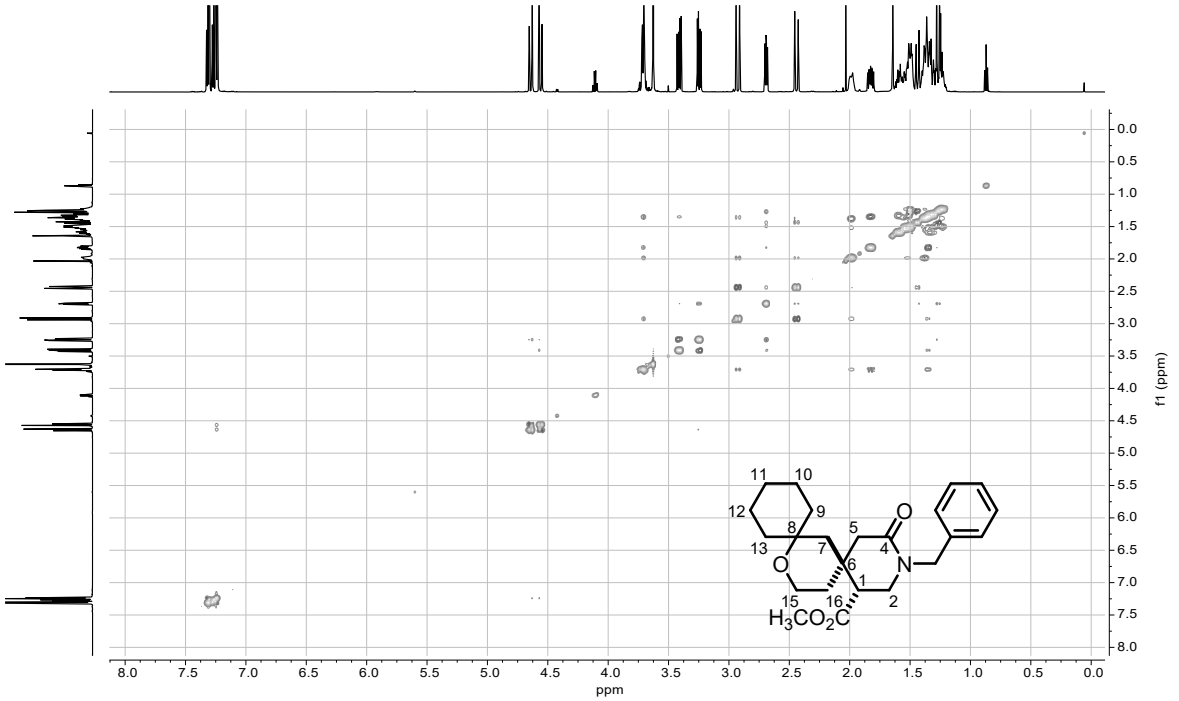
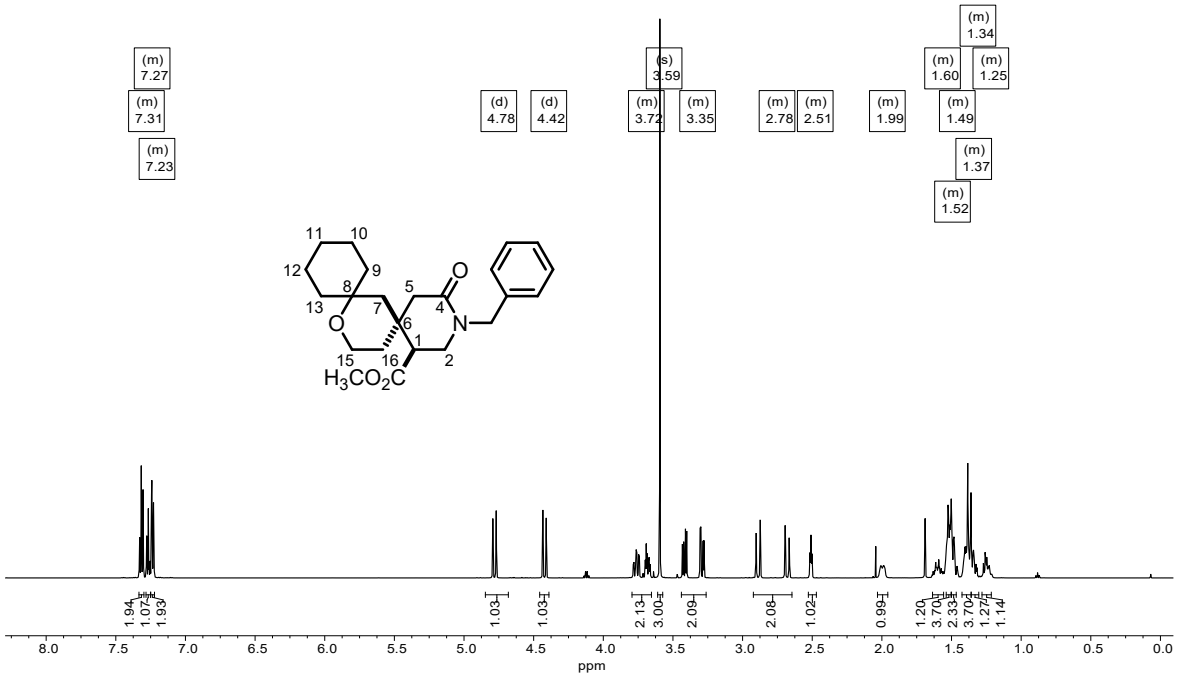
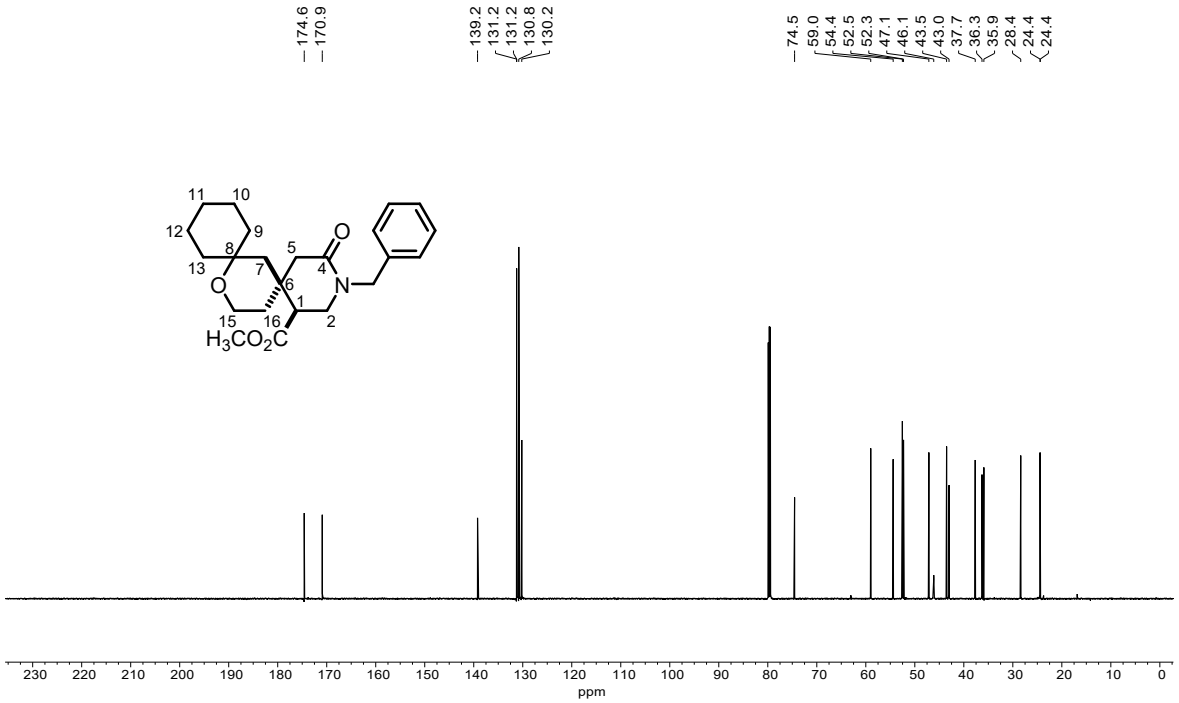


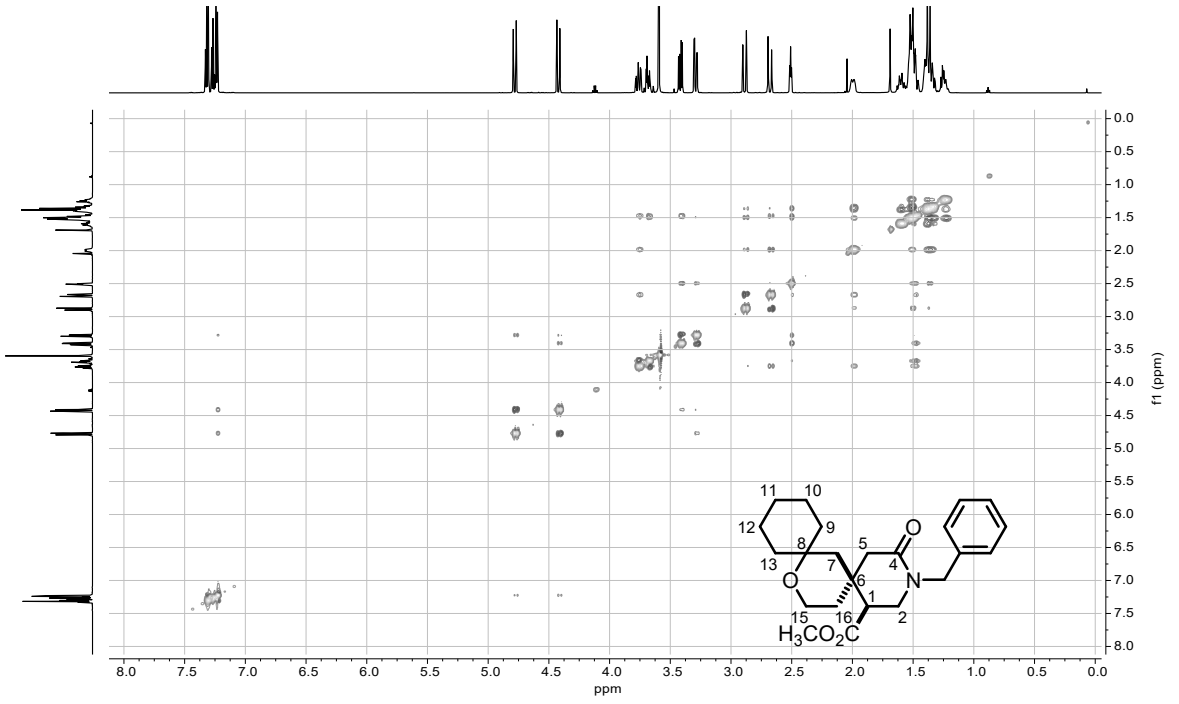
NOESY spectrum of **18a** in $CDCl_3$.



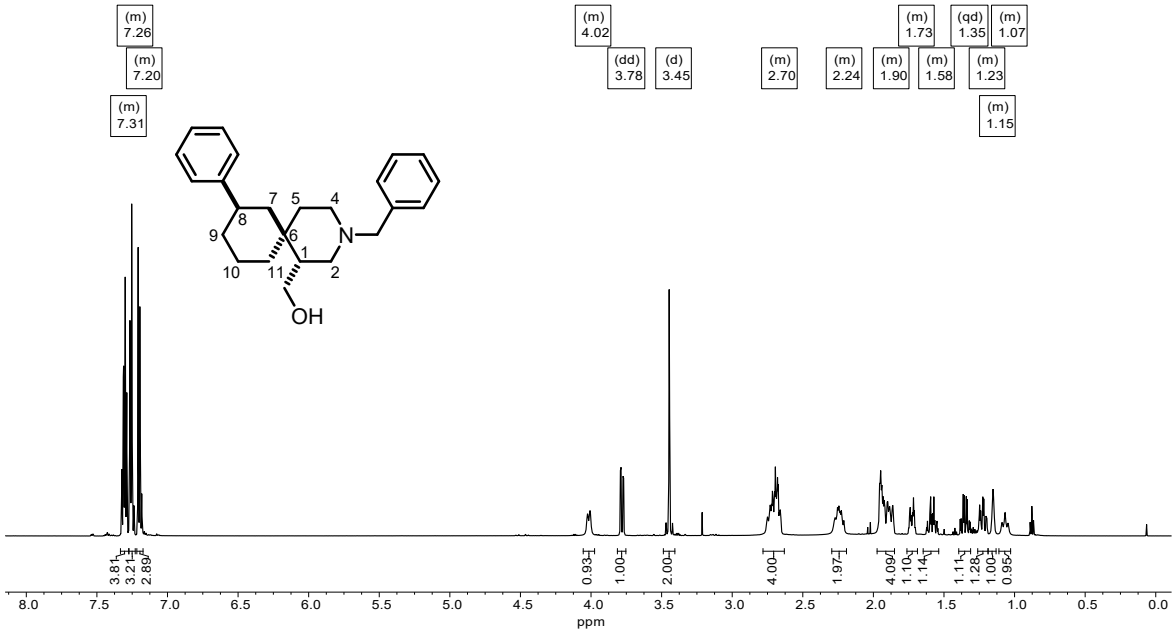
^{1}H NMR spectrum of **18b** in $CDCl_3$.



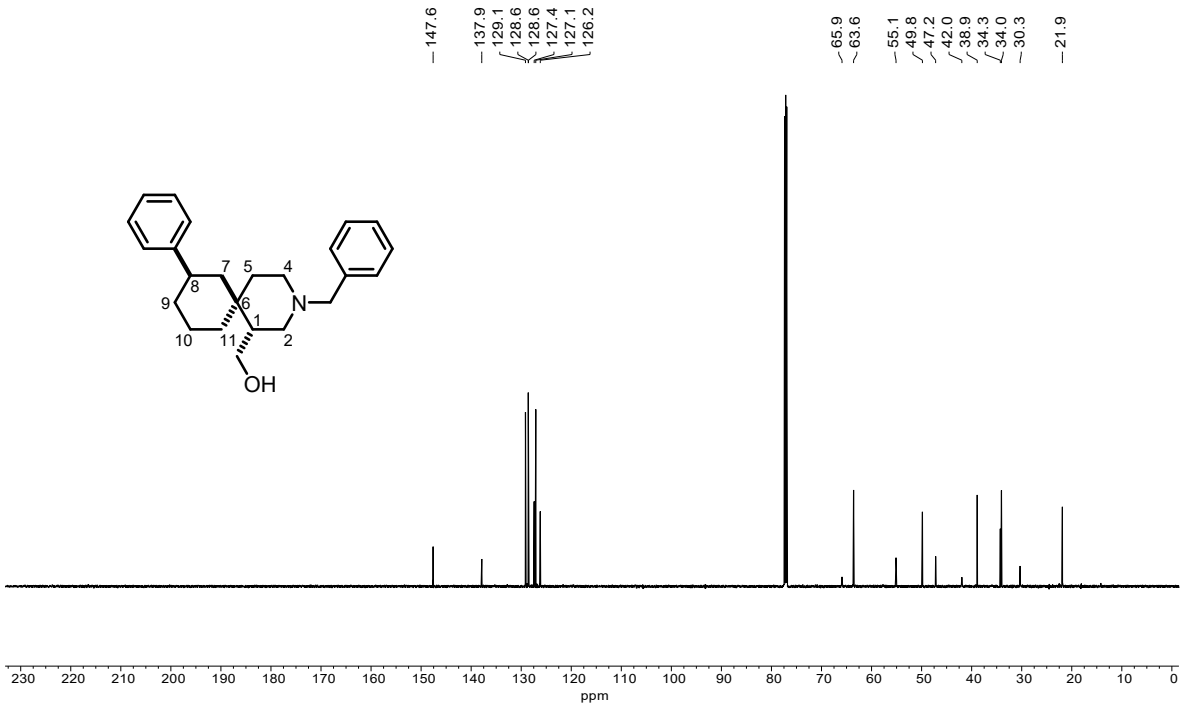
^{13}C NMR spectrum of **18b** in $CDCl_3$.



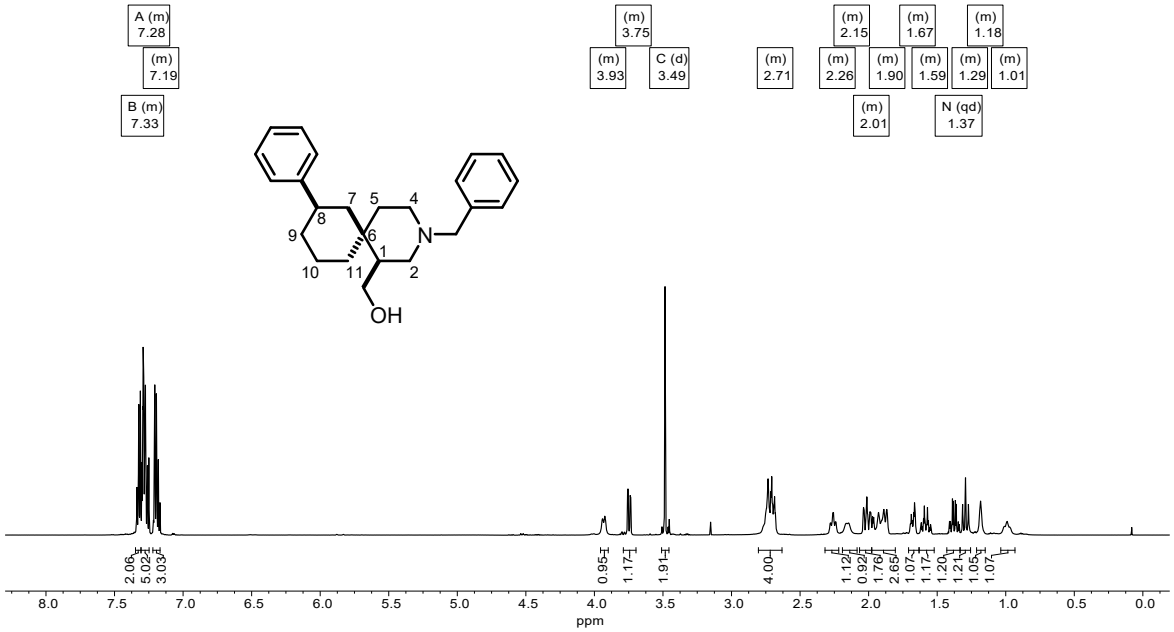
NOESY spectrum of **18b** in $CDCl_3$.



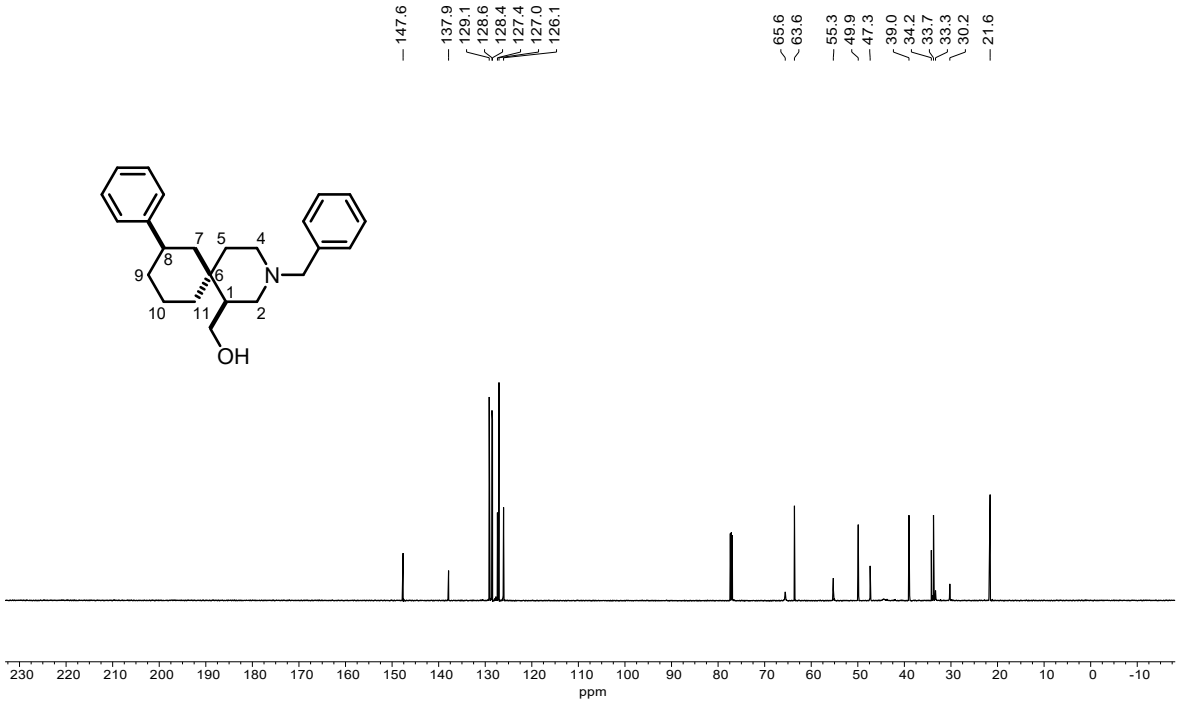
^{1}H NMR spectrum of **21a** in $CDCl_3$.



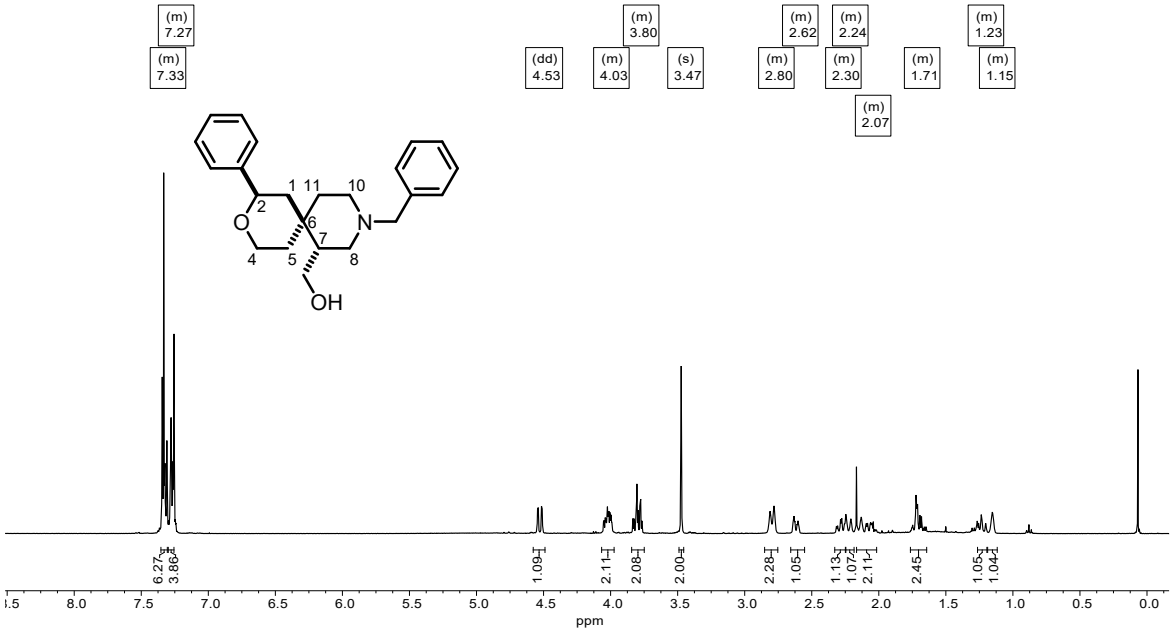
^{13}C NMR spectrum of **21a** in $CDCl_3$.



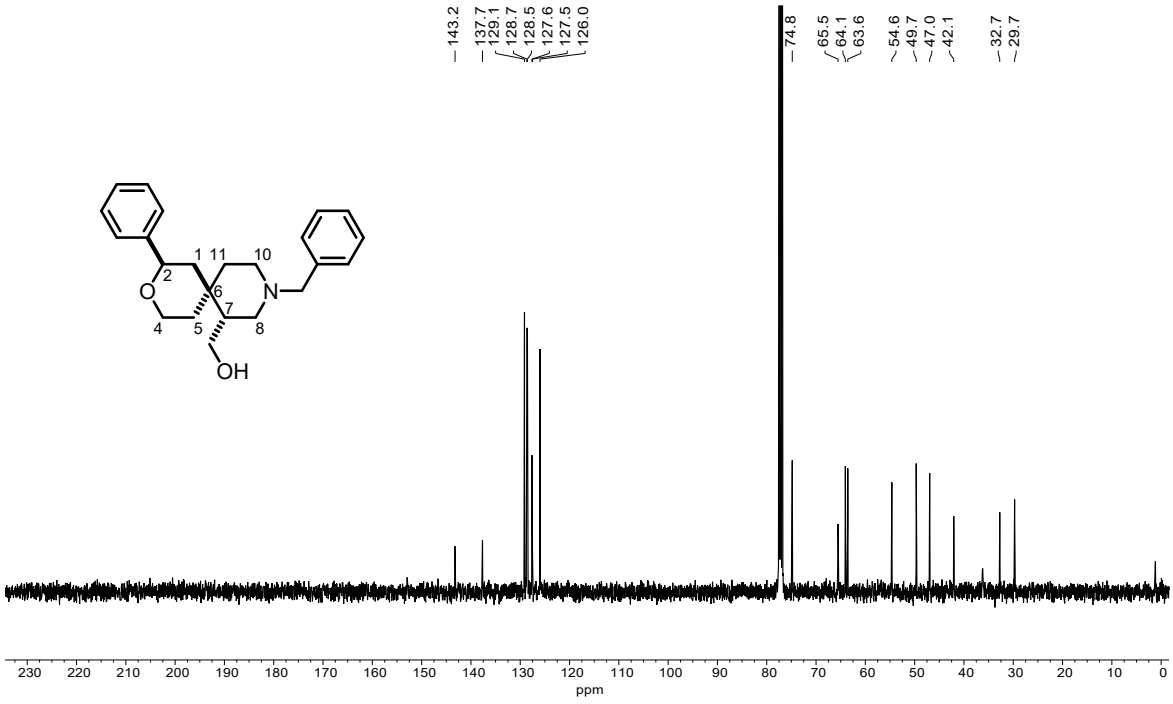
^{1}H NMR spectrum of **21b** in $CDCl_3$.



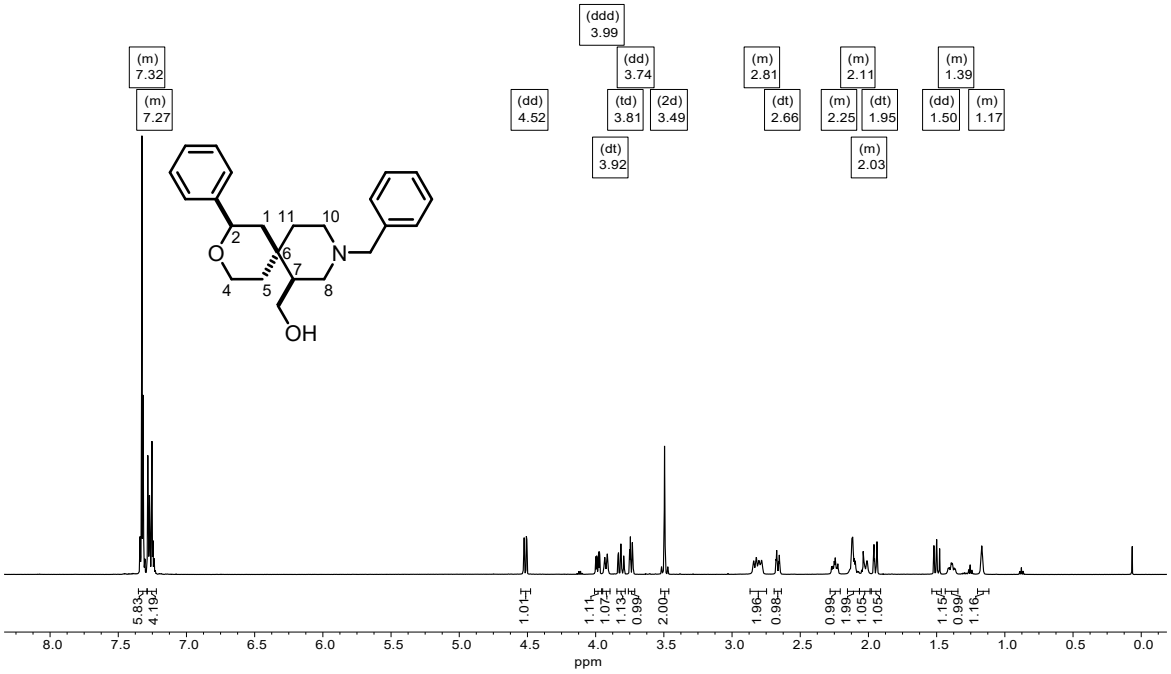
^{13}C NMR spectrum of **21b** in $CDCl_3$.



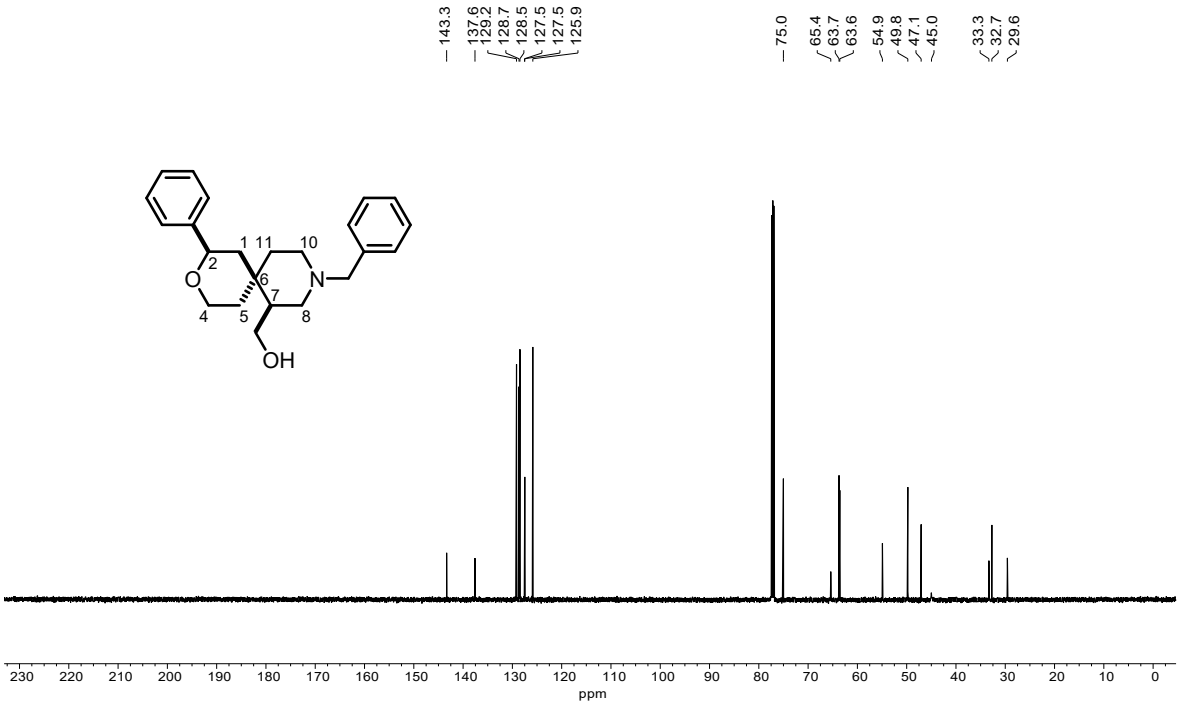
^{1}H NMR spectrum of **22a** in $CDCl_3$.



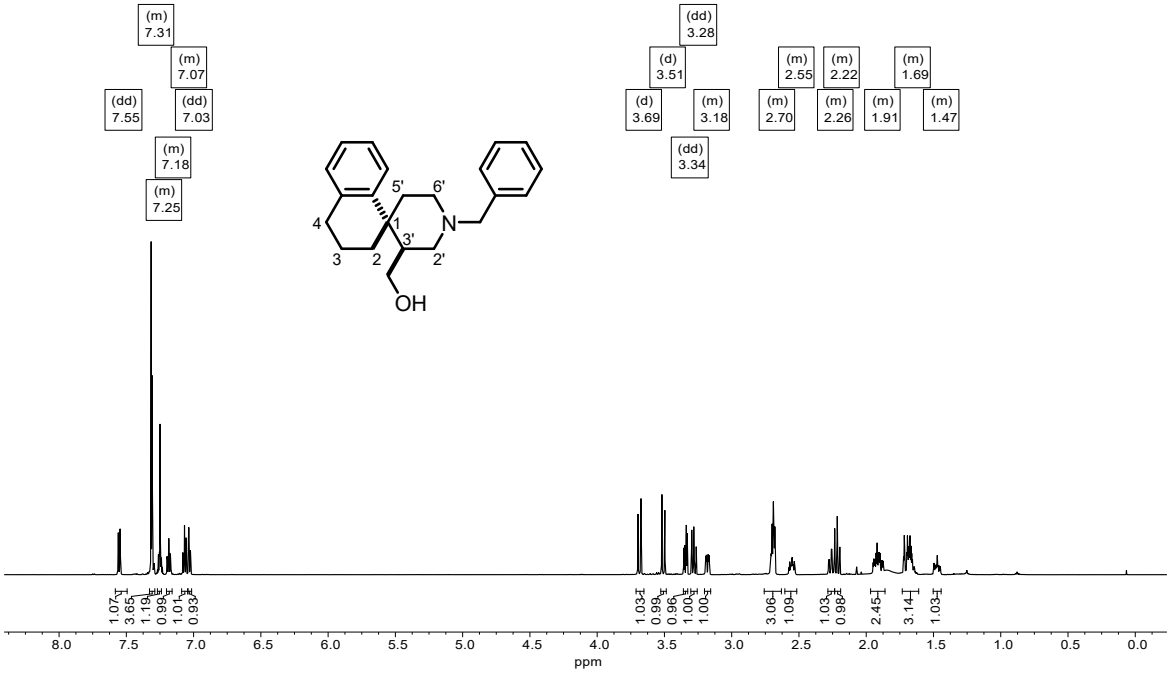
^{13}C NMR spectrum of **22a** in $CDCl_3$.



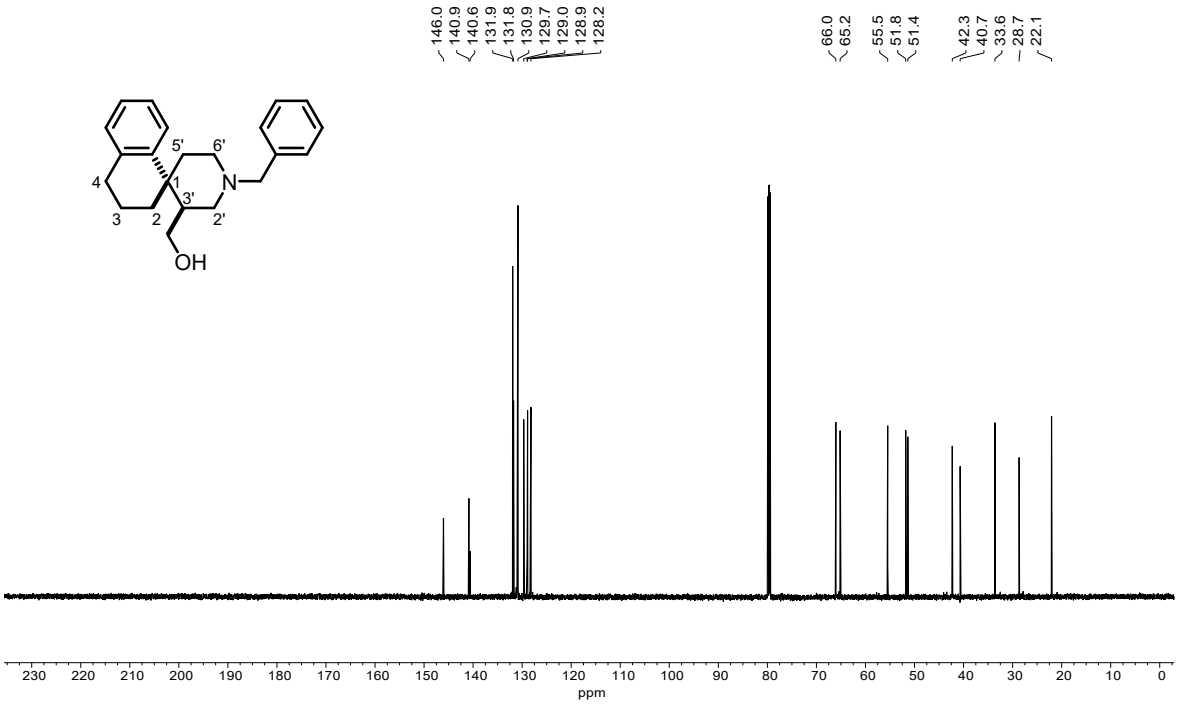
^{1}H NMR spectrum of **22b** in $CDCl_3$.



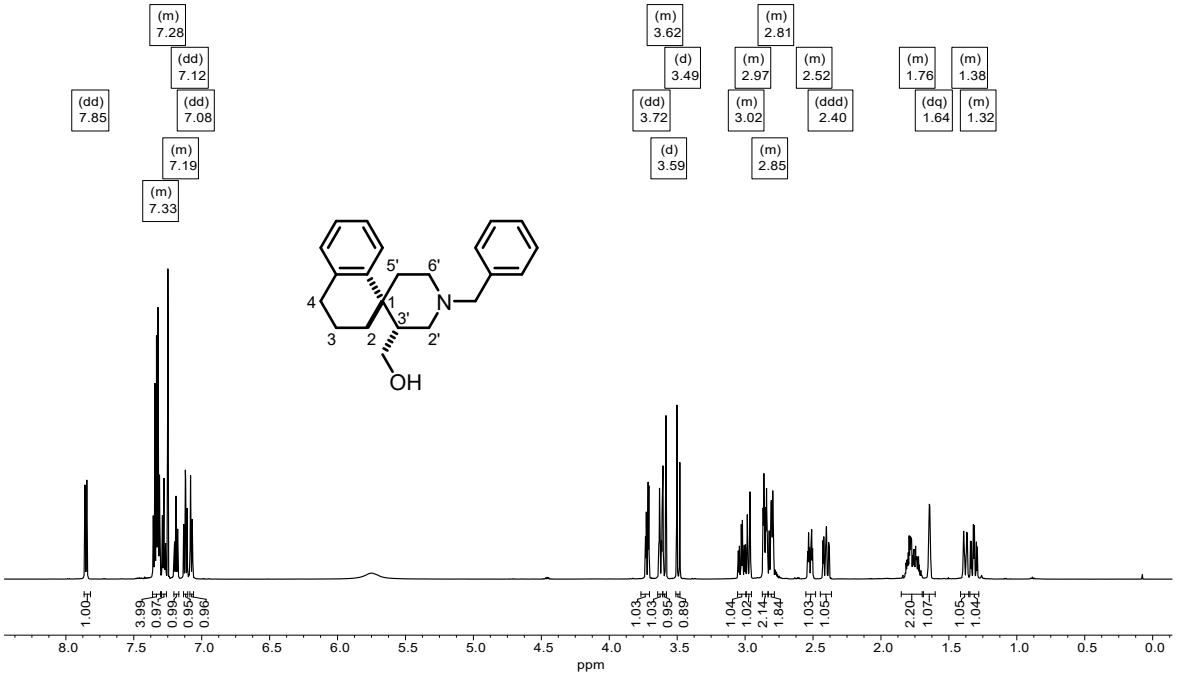
^{13}C NMR spectrum of **22b** in $CDCl_3$.



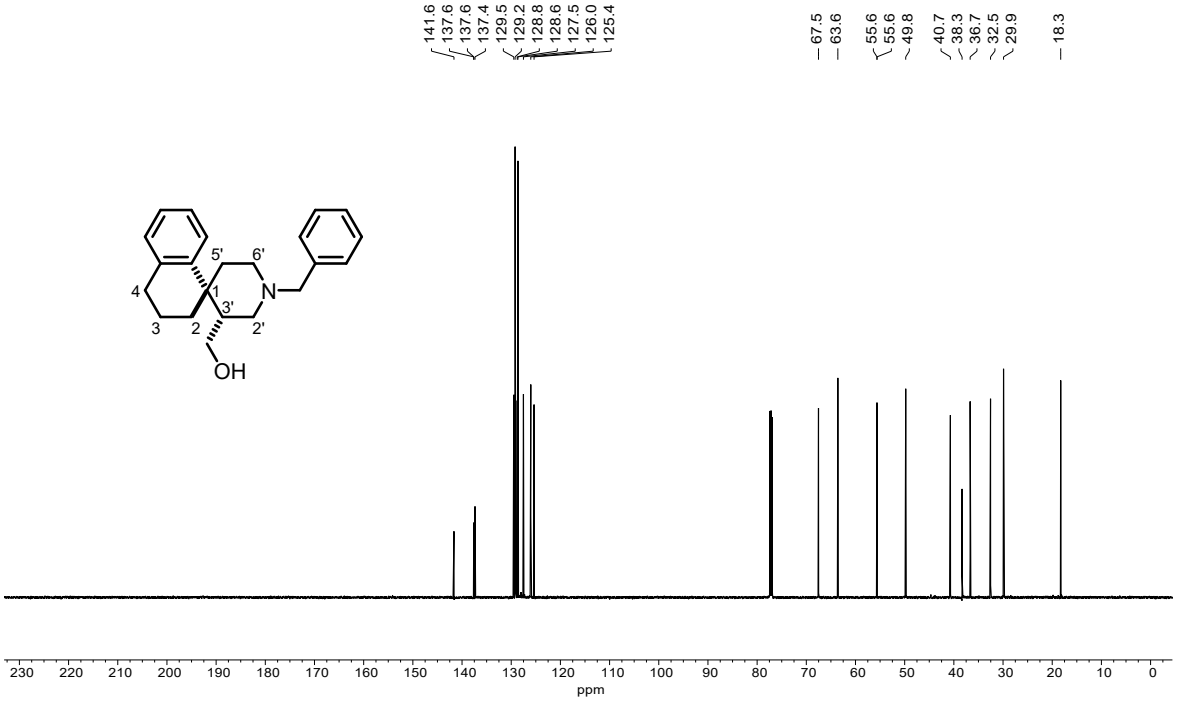
^{1}H NMR spectrum of **24a** in $CDCl_3$.



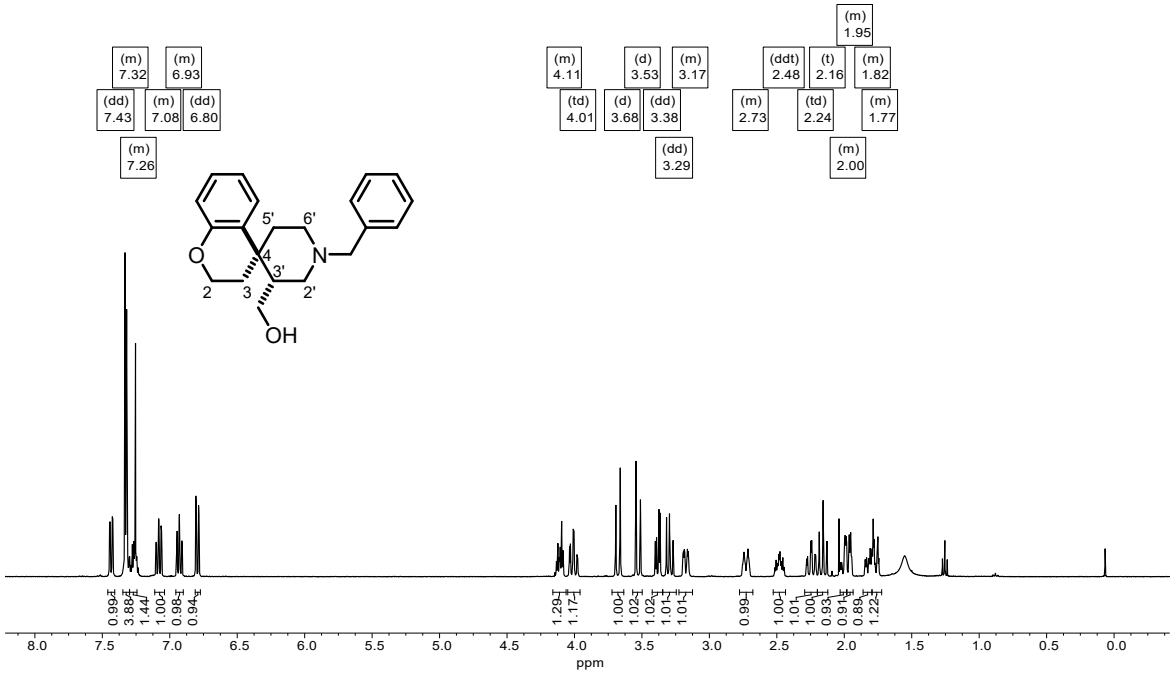
^{13}C NMR spectrum of **24a** in $CDCl_3$.



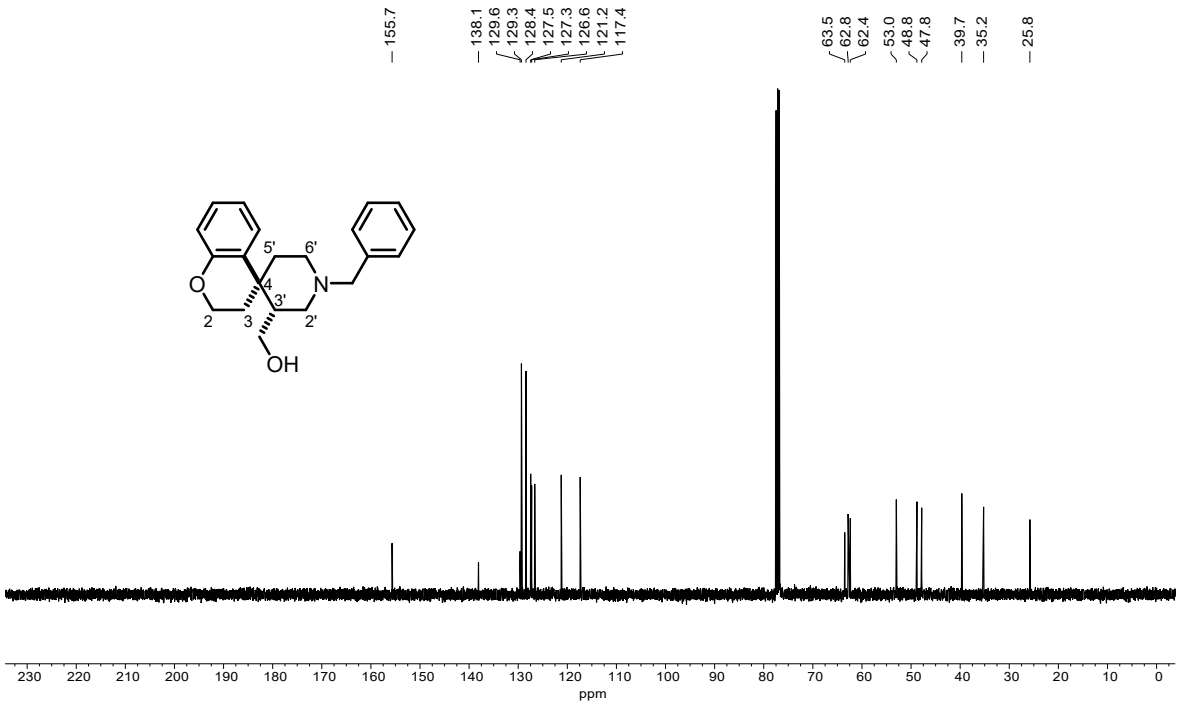
^{1}H NMR spectrum of **24b** in $CDCl_3$.



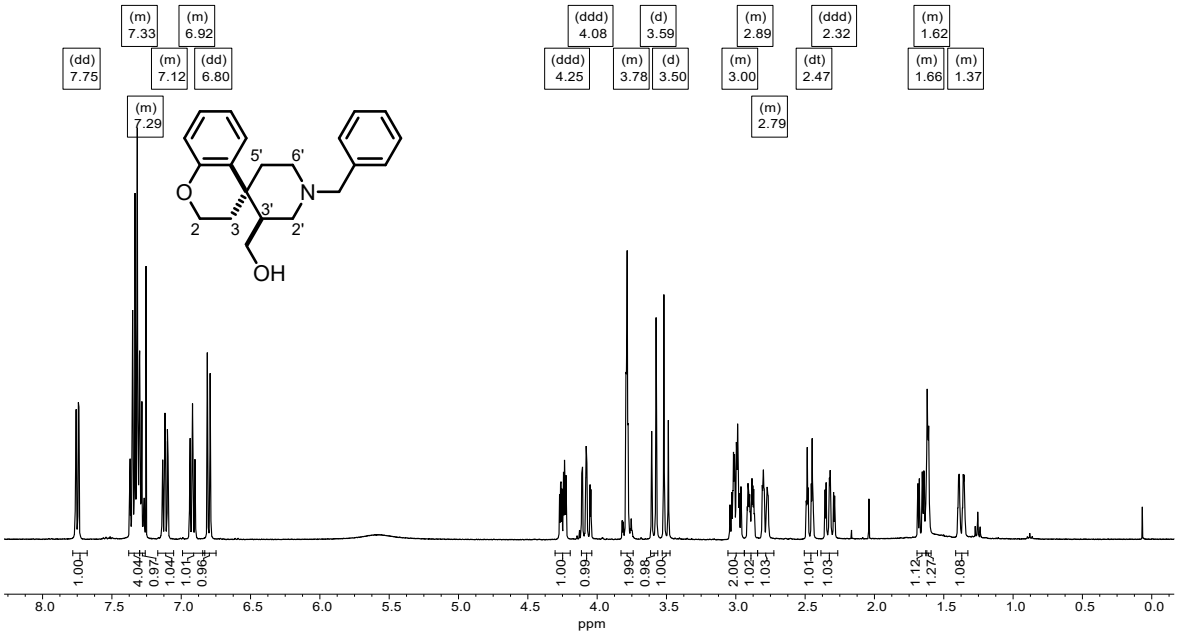
^{13}C NMR spectrum of **24b** in $CDCl_3$.



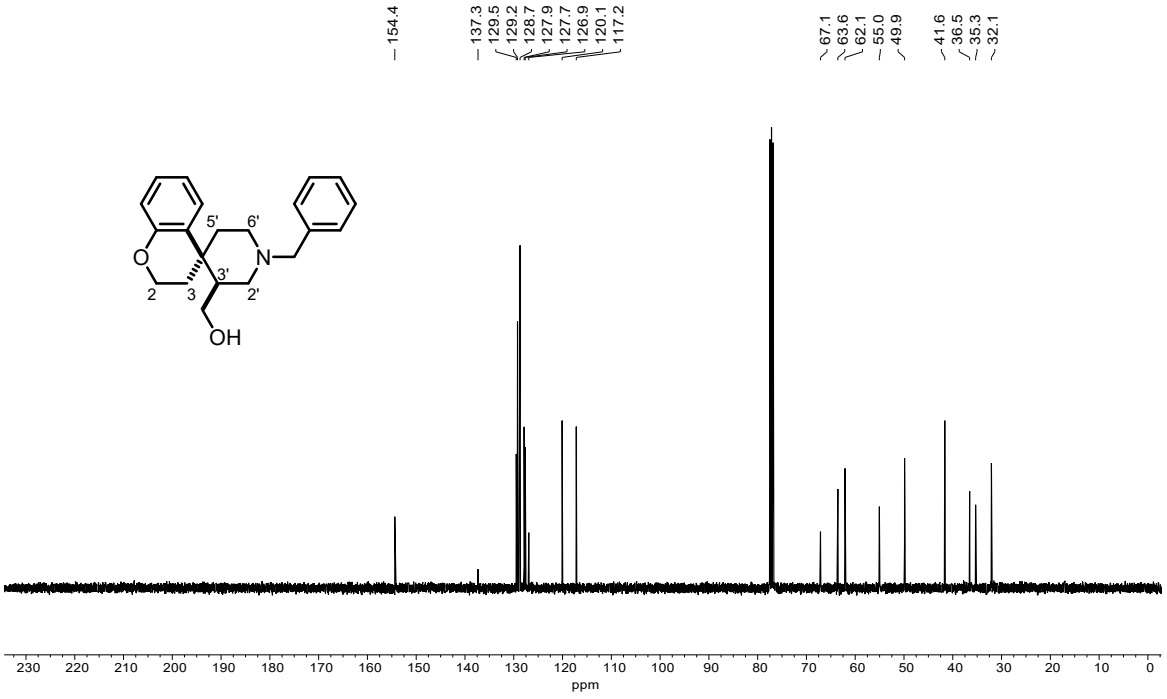
^{1}H NMR spectrum of **25a** in $CDCl_3$.



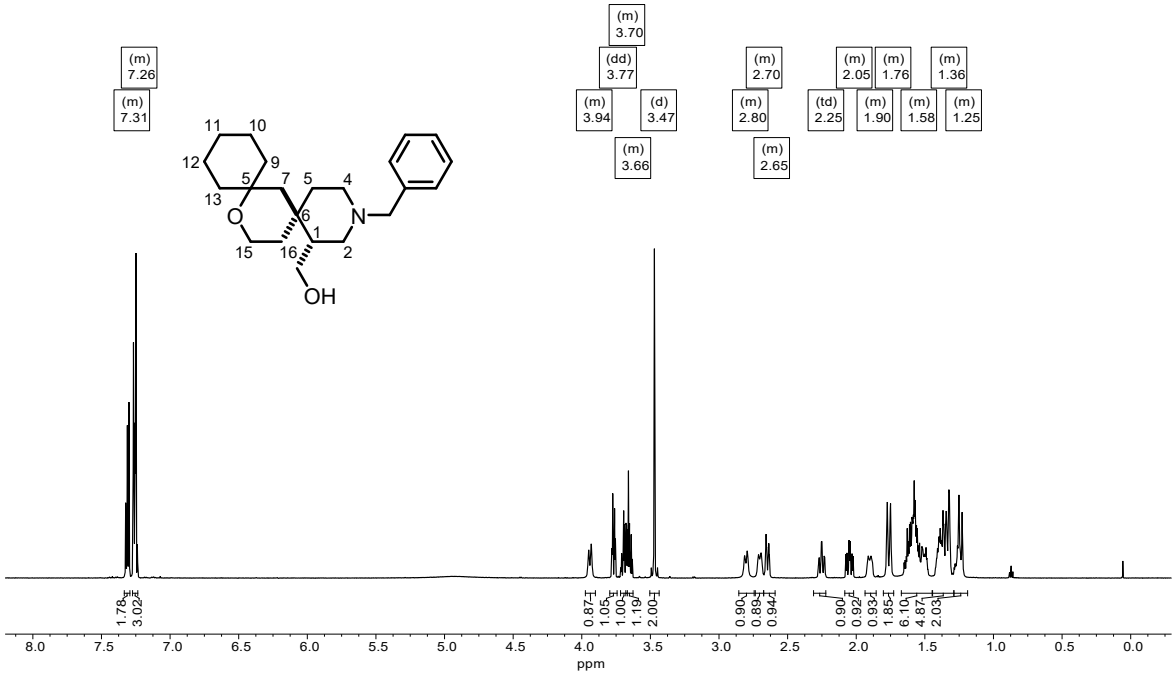
^{13}C NMR spectrum of **25a** in $CDCl_3$.



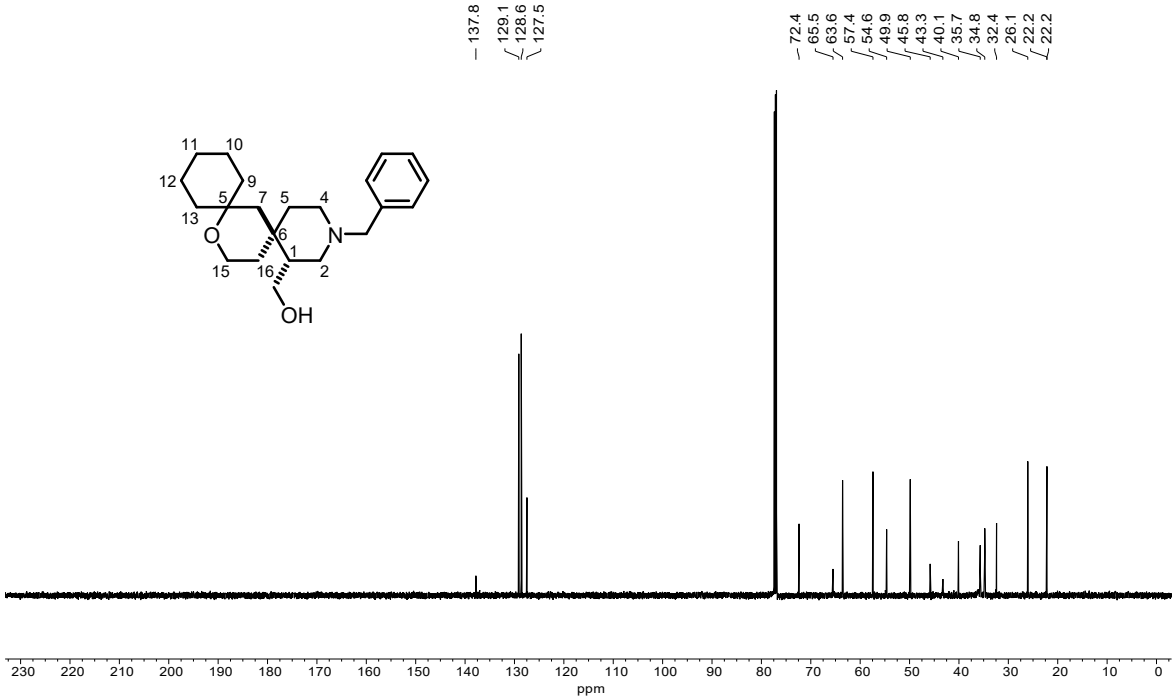
^{1}H NMR spectrum of **25b** in $CDCl_3$.



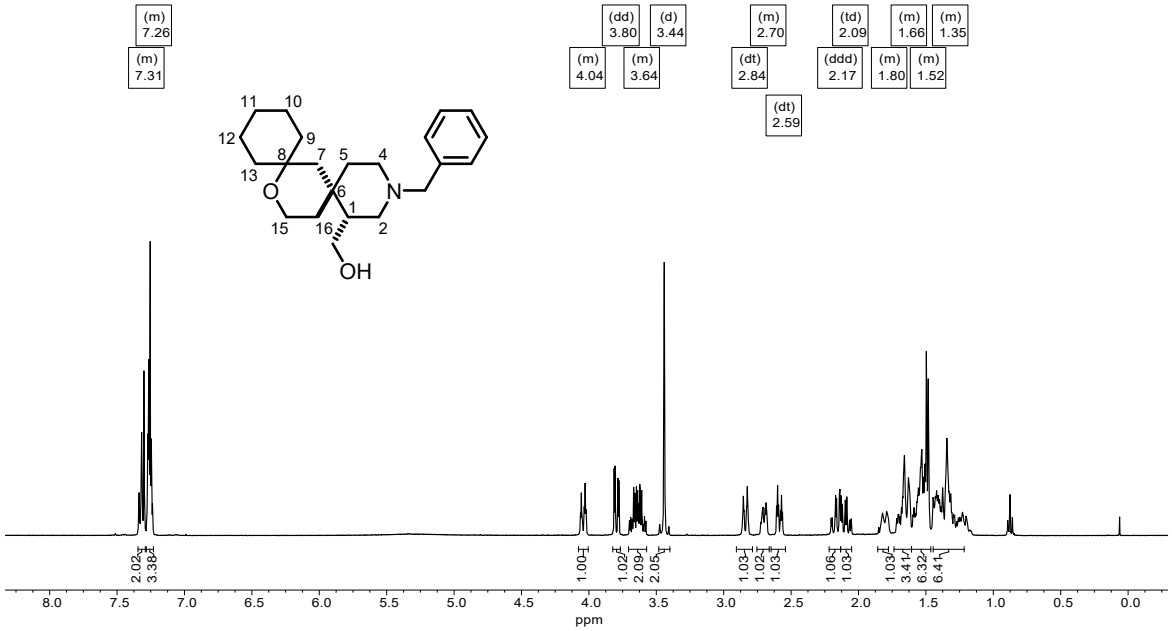
^{13}C NMR spectrum of **25b** in $CDCl_3$.



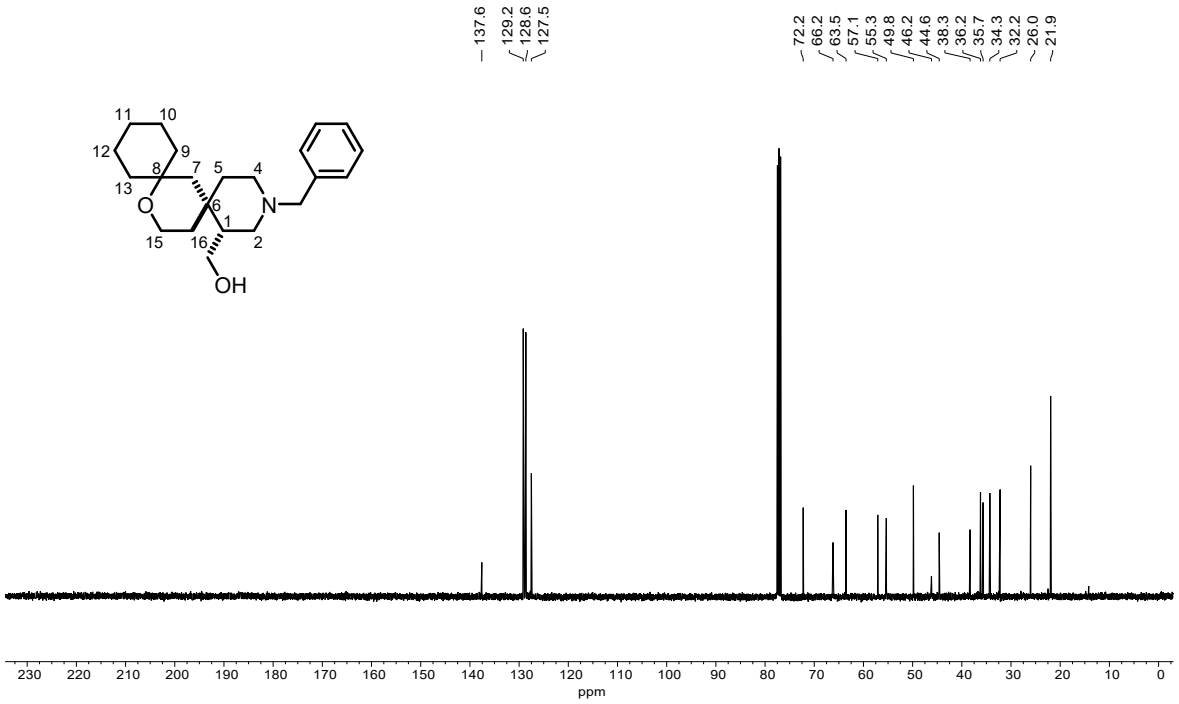
^{1}H NMR spectrum of **23a** in $CDCl_3$.



^{13}C NMR spectrum of **23a** in $CDCl_3$.



^{1}H NMR spectrum of **23b** in $CDCl_3$.



^{13}C NMR spectrum of **23b** in $CDCl_3$.

HPLC purity measurements

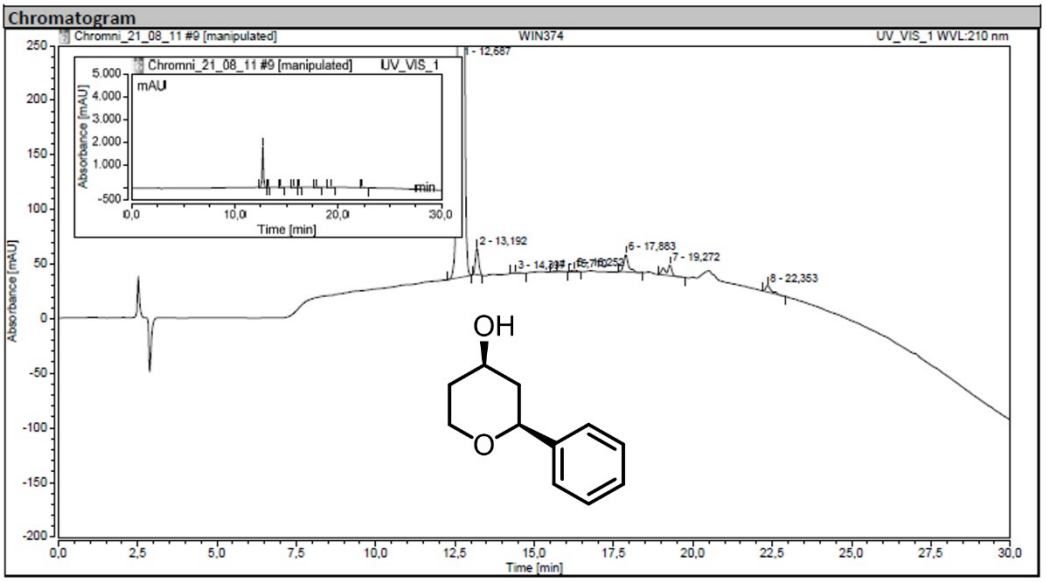
cis-2-Phenyltetrahydro-2*H*-pyran-4-ol

Chromatogram and Results

Injection Details

Injection Name:	**WIN374**	*Run Time (min):*	**30,00**
Vial Number:	**GA7**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Aug.21 17:01**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12,687	247,505	1786,426	96,25	96,80	n.a.
2		13,192	2,867	24,152	1,11	1,31	n.a.
3		14,397	0,191	0,789	0,07	0,04	n.a.
4		15,710	0,258	0,856	0,10	0,05	n.a.
5		16,252	0,249	1,187	0,10	0,06	n.a.
6		17,883	2,775	16,352	1,08	0,89	n.a.
7		19,272	2,177	9,768	0,85	0,53	n.a.
8		22,353	1,132	6,015	0,44	0,33	n.a.
Total:			**257,155**	**1845,546**	**100,00**	**100,00**	

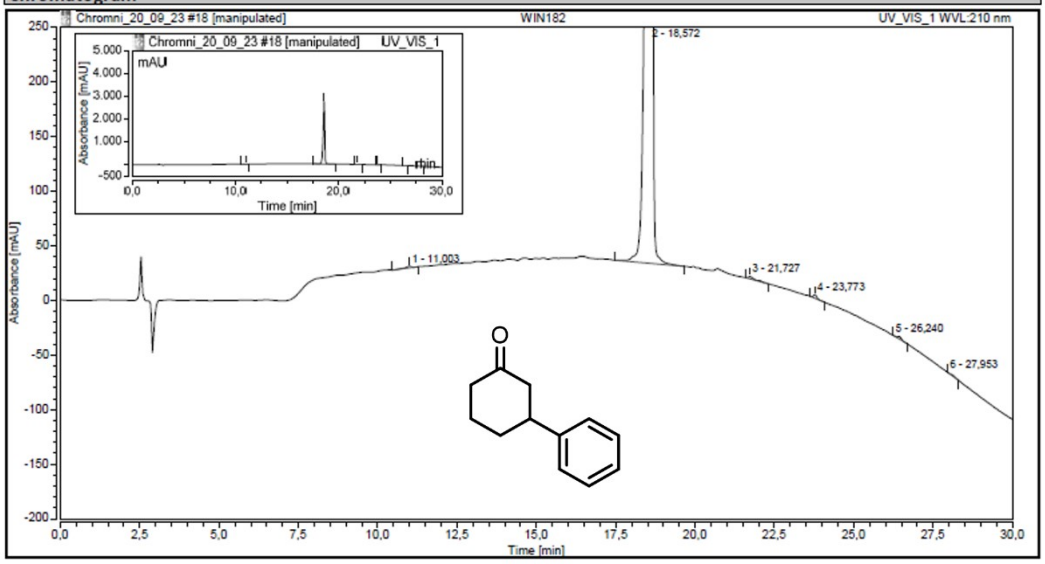
(*RS*)-3-Phenylcyclohexan-1-one (3)

Chromatogram and Results

Injection Details

Injection Name:	**WIN182**	*Run Time (min):*	**30,00**
Vial Number:	**GB7**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**23.Sep.20 20:23**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11,003	0,271	1,618	0,06	0,06	n.a.
2		18,572	441,004	2740,328	99,62	99,73	n.a.
3		21,727	0,508	2,242	0,11	0,08	n.a.
4		23,773	0,423	3,517	0,10	0,13	n.a.
5		26,240	0,332	0,000	0,07	0,00	n.a.
6		27,953	0,147	0,000	0,03	0,00	n.a.
Total:			**442,685**	**2747,705**	**100,00**	**100,00**	

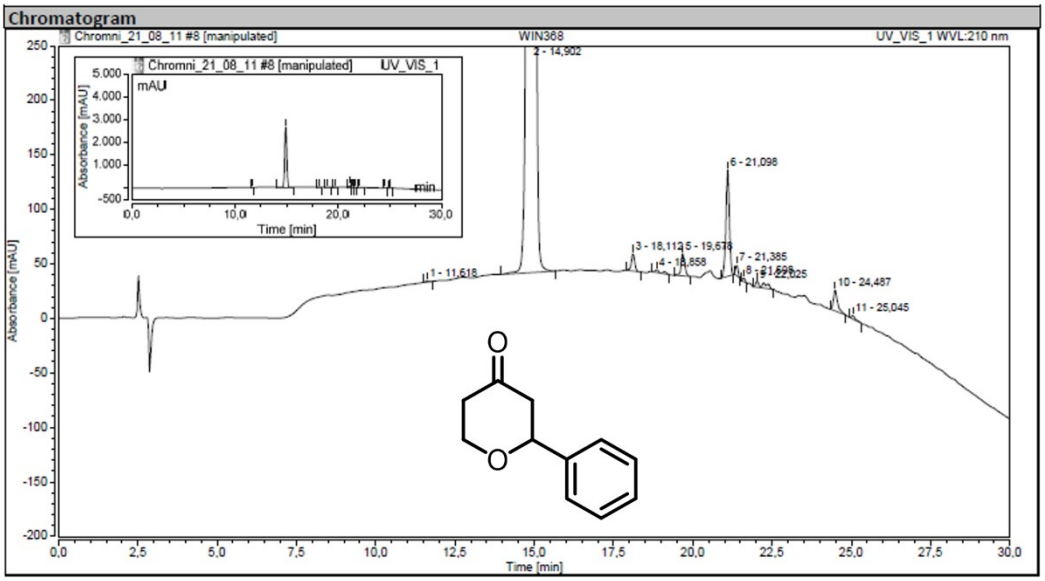
(*RS*)-2-Phenyltetrahydropyran-4-one (9)

Chromatogram and Results

Injection Details

Injection Name:	**WIN368**	*Run Time (min):*	**30,00**
Vial Number:	**GA6**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Aug.21 16:20**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		11,618	0,115	1,006	0,02	0,04	n.a.
2		14,902	577,110	2644,677	96,04	93,65	n.a.
3		18,112	1,965	16,148	0,33	0,57	n.a.
4		18,858	0,539	2,519	0,09	0,09	n.a.
5		19,678	2,745	20,413	0,46	0,72	n.a.
6		21,098	12,340	97,800	2,05	3,46	n.a.
7		21,385	0,914	9,859	0,15	0,35	n.a.
8		21,598	0,332	3,365	0,06	0,12	n.a.
9		22,025	1,582	5,714	0,26	0,20	n.a.
10		24,487	2,859	19,341	0,48	0,68	n.a.
11		25,045	0,432	3,021	0,07	0,11	n.a.
Total:			**600,932**	**2823,865**	**100,00**	**100,00**	

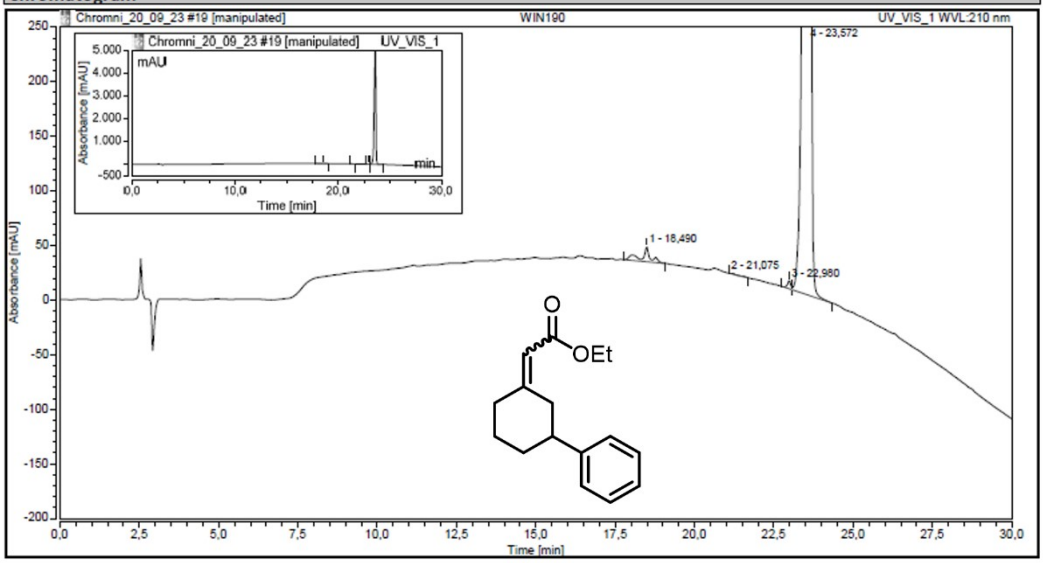
Ethyl (*RS*,*E*)-2-(3-phenylcyclohexyliden)acetate ((*E*)-4) and ethyl (*RS*,*Z*)-2-(3-phenylcyclohexyliden)acetate ((*Z*)-4)

Chromatogram and Results

Injection Details

Injection Name:	**WIN190**	*Run Time (min):*	**30,00**
Vial Number:	**GB8**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**23.Sep.20 21:04**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18,490	4,364	14,056	0,54	0,28	n.a.
2		21,075	0,154	0,000	0,02	0,00	n.a.
3		22,980	0,927	7,800	0,11	0,16	n.a.
4		23,572	806,080	4995,366	99,33	99,56	n.a.
Total:			**811,525**	**5017,221**	**100,00**	**100,00**	

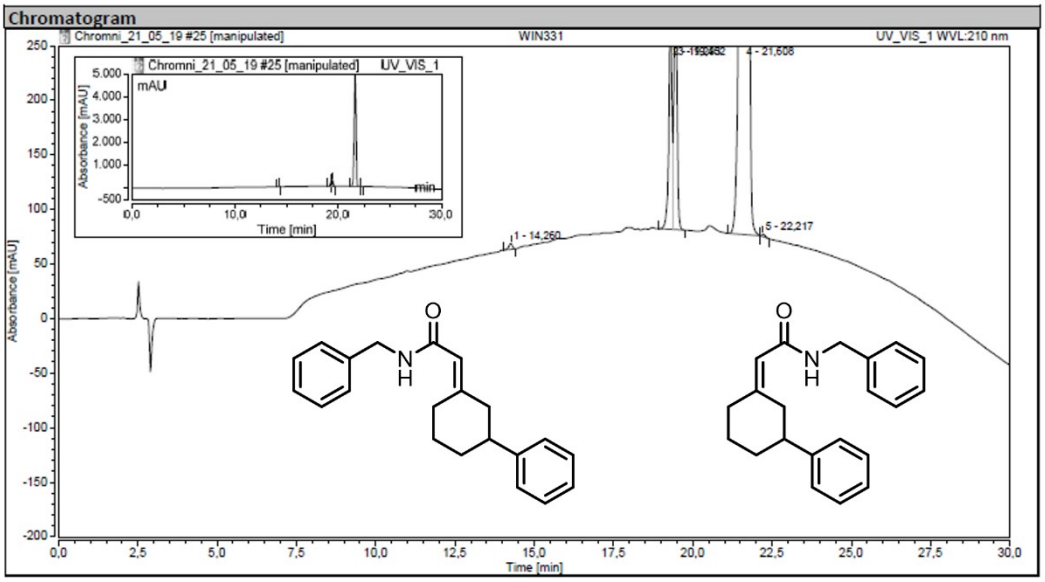
(*RS*,*E*)-*N*-Benzyl-2-(3-phenylcyclohexyliden)acetamide ((*E*)-6) and (*RS*,*Z*)-*N*-benzyl-2-(3-phenylcyclohexyliden)acetamide ((*Z*)-6)

Chromatogram and Results

Injection Details

Injection Name:	**WIN331**	*Run Time (min):*	**30,00**
Vial Number:	**GC5**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**20.Mai.21 03:03**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14,260	0,710	5,425	0,06	0,10	n.a.
2		19,293	22,319	200,355	1,94	3,71	n.a.
3		19,452	28,063	268,893	2,44	4,98	n.a.
4		21,608	1098,168	4922,996	95,53	91,16	n.a.
5		22,217	0,292	2,448	0,03	0,05	n.a.
Total:			**1149,553**	**5400,117**	**100,00**	**100,00**	

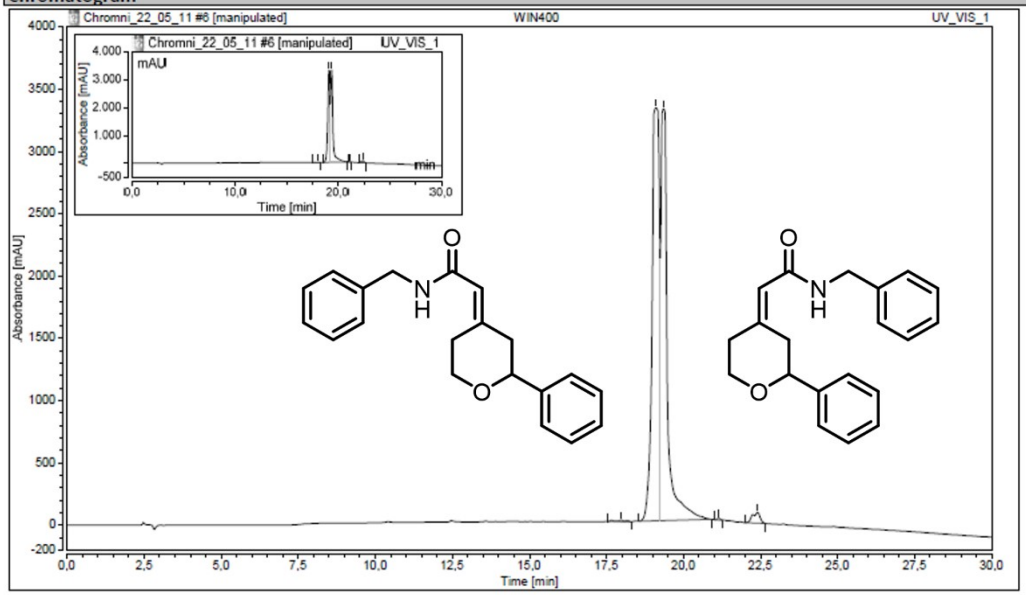
(*RS*,*E*)-*N*-Benzyl-2-(2-phenyltetrahydro-4*H*-pyran-4-ylidene)acetamide ((*E*)-13) and (*RS*,*Z*)-*N*-benzyl-2-(2-phenyltetrahydro-4*H*-pyran-4-ylidene)acetamide ((*Z*)-13)

Chromatogram and Results

Injection Details

Injection Name:	**WIN400**	*Run Time (min):*	**30,00**
Vial Number:	**GA2**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Mai.22 18:06**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17,982	4,108	12,356	0,23	0,18	n.a.
2		19,102	901,219	3316,019	51,14	49,25	n.a.
3		19,357	831,063	3304,252	47,16	49,08	n.a.
4		21,140	1,511	13,739	0,09	0,20	n.a.
5		22,403	24,435	86,555	1,39	1,29	n.a.
Total:			**1762,335**	**6732,921**	**100,00**	**100,00**	

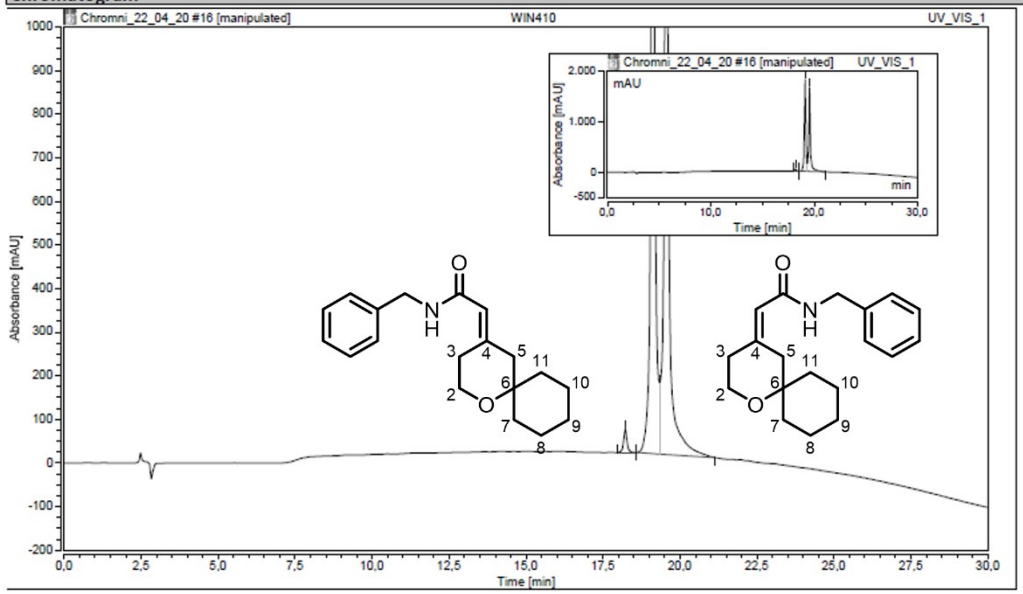
(*E*)-*N*-Benzyl-2-(1-oxaspiro[5.5]undecan-4-ylidene)acetamide ((*E*)-14) and (*Z*)-*N*-benzyl-2-(1-oxaspiro[5.5]undecan-4-ylidene)acetamide ((Z)-14)

Chromatogram and Results

Injection Details

Injection Name:	**WIN410**	*Run Time (min):*	**30,00**
Vial Number:	**GB4**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**21.Apr.22 00:52**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18,220	6,938	53,841	1,22	1,52	n.a.
2		19,112	274,713	1823,383	48,16	51,39	n.a.
3		19,550	288,774	1670,617	50,62	47,09	n.a.
Total:			**570,425**	**3547,841**	**100,00**	**100,00**	

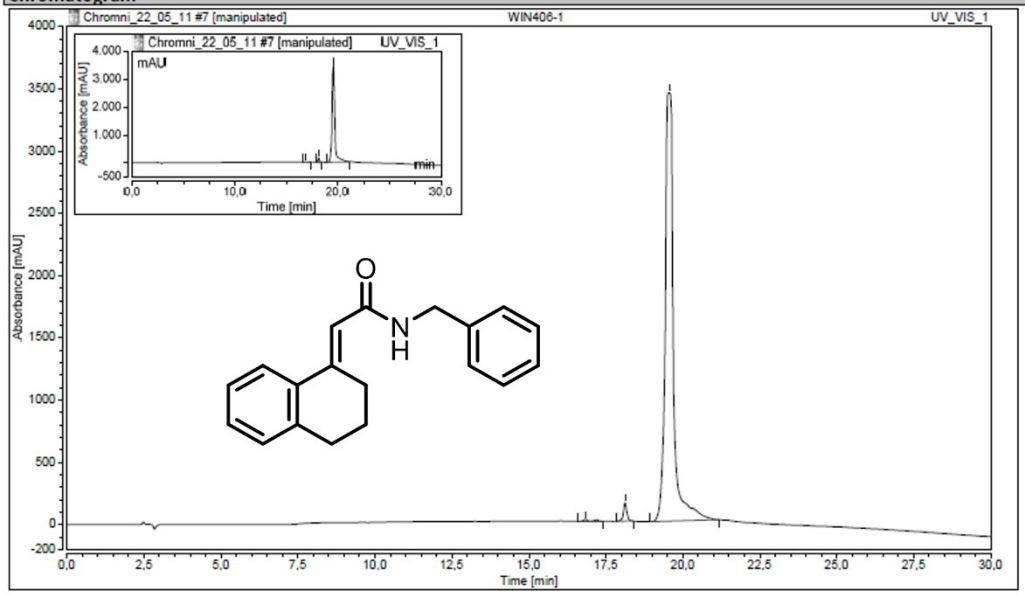
(*E*)-*N*-Benzyl-2-(3,4-dihydronaphthalen-1[2*H*]-yliden)acetamide (15)

Chromatogram and Results

Injection Details

Injection Name:	**WIN406-1**	*Run Time (min):*	**30,00**
Vial Number:	**GA3**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Mai.22 18:47**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16,832	3,509	14,700	0,32	0,41	n.a.
2		18,123	19,105	148,955	1,74	4,13	n.a.
3		19,557	1077,956	3443,196	97,95	95,46	n.a.
Total:			**1100,570**	**3606,851**	**100,00**	**100,00**	

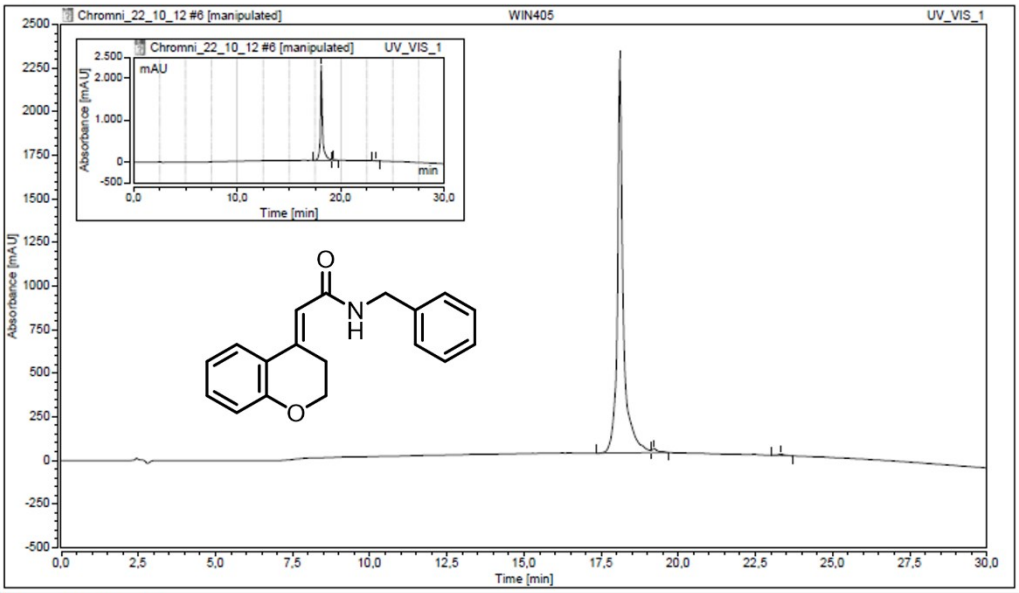
(*E*)-*N*-Benzyl-2-(2,3-dihydro-1-benzopyran-4-yliden)acetamide (16)

Chromatogram and Results

Injection Details

Injection Name:	**WIN405**	*Run Time (min):*	**30,00**
Vial Number:	**GA3**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**12.Okt.22 18:14**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18,103	492,276	2258,700	98,54	98,58	n.a.
2		19,215	5,523	24,029	1,11	1,05	n.a.
3		23,320	1,792	8,581	0,36	0,37	n.a.
Total:			**499,592**	**2291,310**	**100,00**	**100,00**	

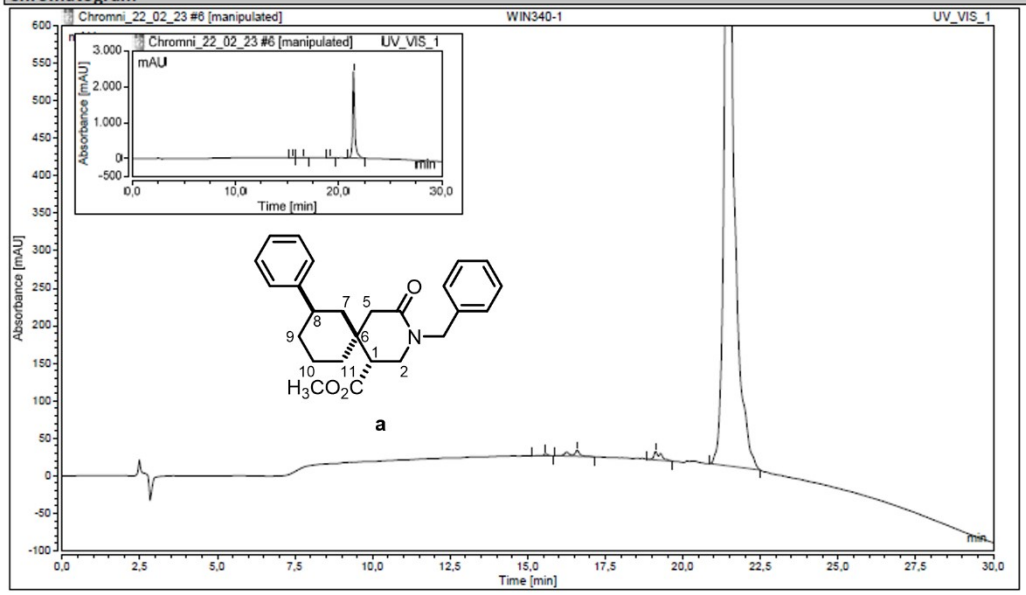
Methyl (1*RS*,6*SR*,8*RS*)-3-benzyl-4-oxo-8-phenyl-3-azaspiro[5.5]undecane-1-carboxylate (8a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN340-1**	*Run Time (min):*	**30,00**
Vial Number:	**GA4**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**23.Feb.22 18:57**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15,573	0,537	3,186	0,10	0,13	n.a.
2		16,590	2,686	8,615	0,49	0,35	n.a.
3		19,118	2,870	11,519	0,52	0,47	n.a.
4		21,448	543,416	2411,539	98,89	99,04	n.a.
Total:			**549,510**	**2434,860**	**100,00**	**100,00**	

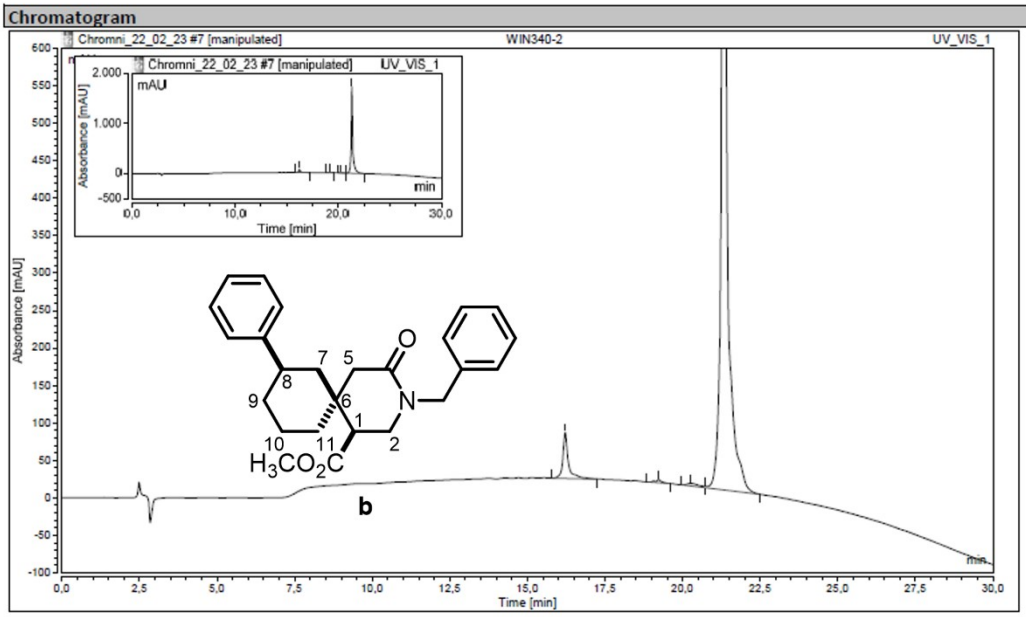
Methyl (1*SR*,6*SR*,8*RS*)-3-benzyl-4-oxo-8-phenyl-3-azaspiro[5.5]undecane-1-carboxylate (8b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN340-2**	*Run Time (min):*	**30,00**
Vial Number:	**GA5**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**23.Feb.22 19:38**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16,218	12,496	61,365	4,00	3,43	n.a.
2		19,228	0,910	4,593	0,29	0,26	n.a.
3		20,257	1,513	3,252	0,48	0,18	n.a.
4		21,320	297,411	1720,787	95,22	96,13	n.a.
Total:			**312,329**	**1789,996**	**100,00**	**100,00**	

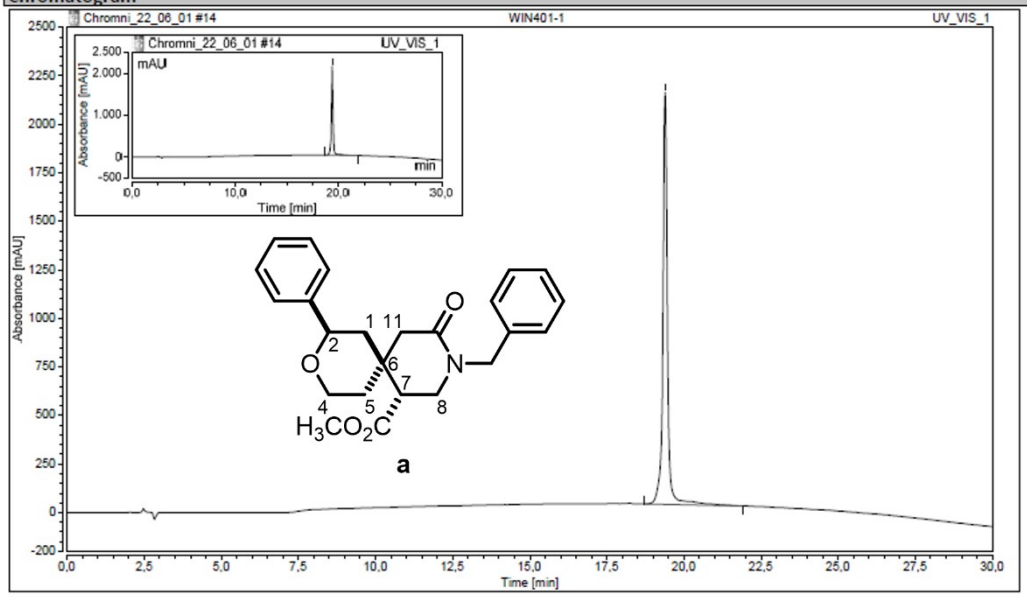
Methyl (2*RS*,6*SR*,7*RS*)-9-benzyl-10-oxo-2-phenyl-3-oxa-9-azaspiro[5.5]undecane-7-carboxylate (17a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN401-1**	*Run Time (min):*	**30,00**
Vial Number:	**GB2**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**01.Jun.22 23:42**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		19,388	366,780	2123,775	100,00	100,00	n.a.
Total:			**366,780**	**2123,775**	**100,00**	**100,00**	

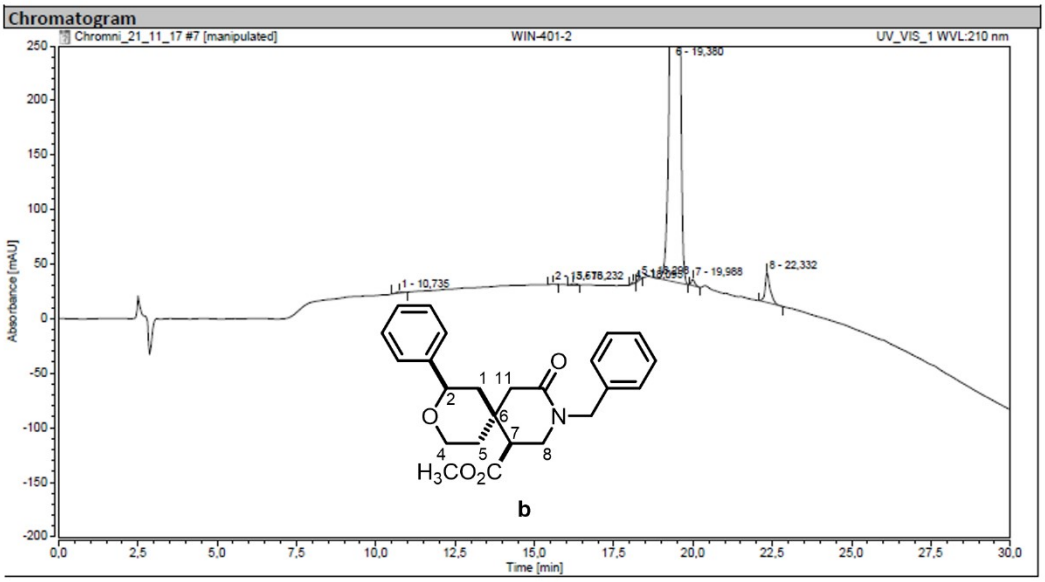
Methyl (2RS,6SR,7SR)-9-benzyl-10-oxo-2-phenyl-3-oxa-9-azaspiro[5.5]undecane-7-carboxylate (17b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN-401-2**	*Run Time (min):*	**30,00**
Vial Number:	**GA5**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**17.Nov.21 16:40**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		10,735	0,271	1,200	0,06	0,06	n.a.
2		15,573	0,107	0,702	0,03	0,03	n.a.
3		16,232	0,236	1,113	0,06	0,05	n.a.
4		18,095	0,140	1,630	0,03	0,07	n.a.
5		18,298	0,248	2,237	0,06	0,10	n.a.
6		19,380	411,565	2138,073	98,37	98,13	n.a.
7		19,988	0,751	5,925	0,18	0,27	n.a.
8		22,332	5,046	27,890	1,21	1,28	n.a.
Total:			**418,364**	**2178,770**	**100,00**	**100,00**	

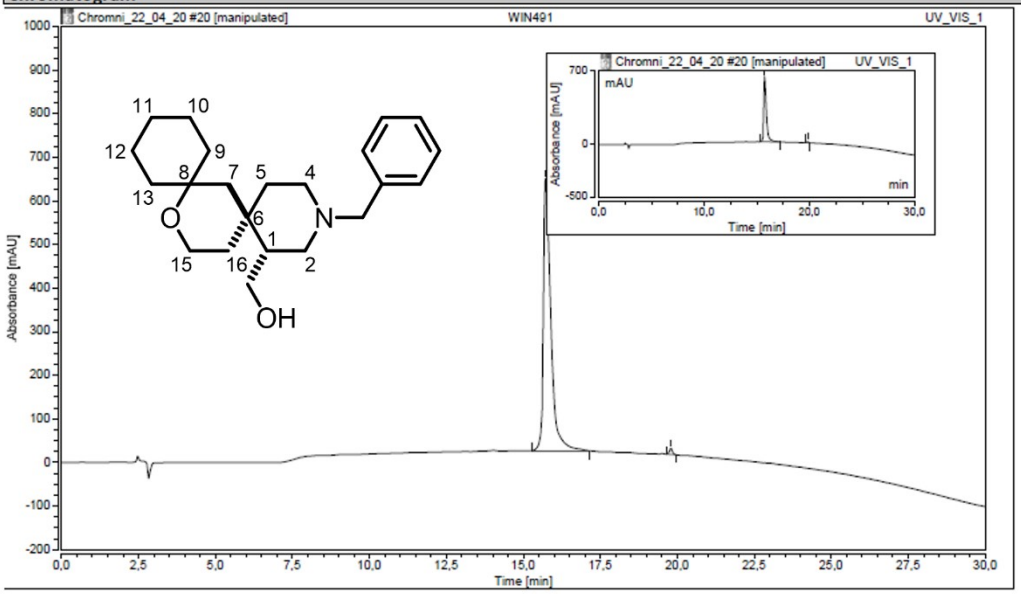
Methyl (1*RS*,6*SR*)-3-benzyl-4-oxo-14-oxa-3-azadispiro[5.1.5^{8}.3^{6}]hexadecane-1-carboxylate (18a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN491**	*Run Time (min):*	**30,00**
Vial Number:	**GB8**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**21.Apr.22 03:35**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15,717	177,304	623,903	99,09	97,73	n.a.
2		19,787	1,634	14,515	0,91	2,27	n.a.
Total:			**178,938**	**638,418**	**100,00**	**100,00**	

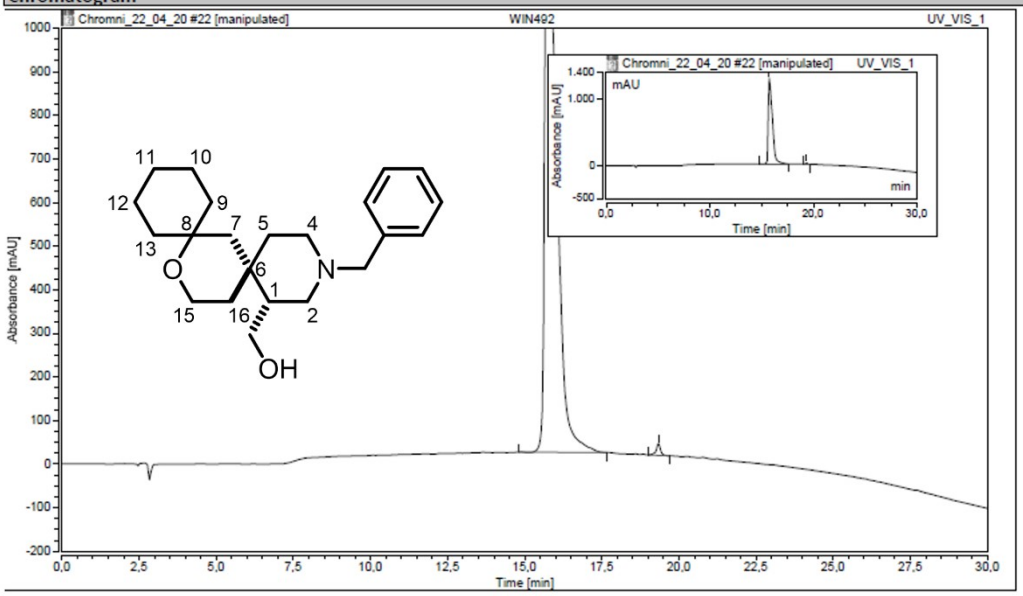
Methyl (1*RS*,6*RS*)-3-benzyl-4-oxo-14-oxa-3-azadispiro[5.1.5^{8}.3^{6}]hexadecane-1-carboxylate (18b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN492**	*Run Time (min):*	**30,00**
Vial Number:	**GC1**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**21.Apr.22 04:57**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15,738	587,874	1293,695	99,27	97,94	n.a.
2		19,330	4,340	27,223	0,73	2,06	n.a.
Total:			**592,214**	**1320,918**	**100,00**	**100,00**	

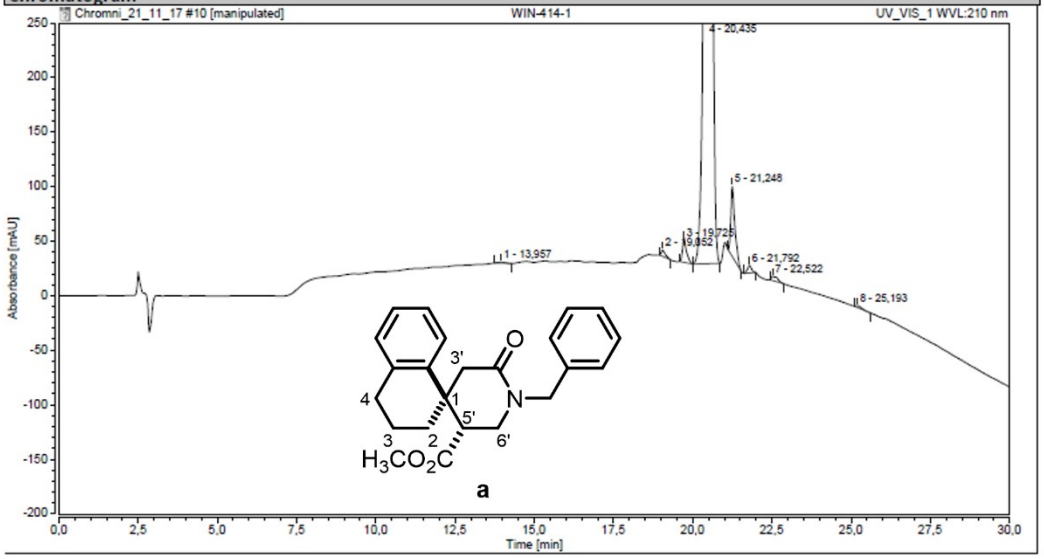
Methyl (1*SR*,5'*RS*)-1'-benzyl-2'-oxo-3,4-dihydro-2H-spiro(naphthalene-1,4'-piperidine)-5'-carboxylate (19a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN-414-1**	*Run Time (min):*	**30,00**
Vial Number:	**GA8**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**17.Nov.21 18:42**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		13,957	0,223	0,888	0,05	0,04	n.a.
2		19,052	0,869	5,879	0,21	0,26	n.a.
3		19,725	3,104	20,767	0,74	0,91	n.a.
4		20,435	406,019	2167,551	96,17	95,39	n.a.
5		21,248	9,518	64,468	2,25	2,84	n.a.
6		21,792	1,056	7,015	0,25	0,31	n.a.
7		22,522	1,015	4,121	0,24	0,18	n.a.
8		25,193	0,386	1,640	0,09	0,07	n.a.
Total:			**422,190**	**2272,329**	**100,00**	**100,00**	

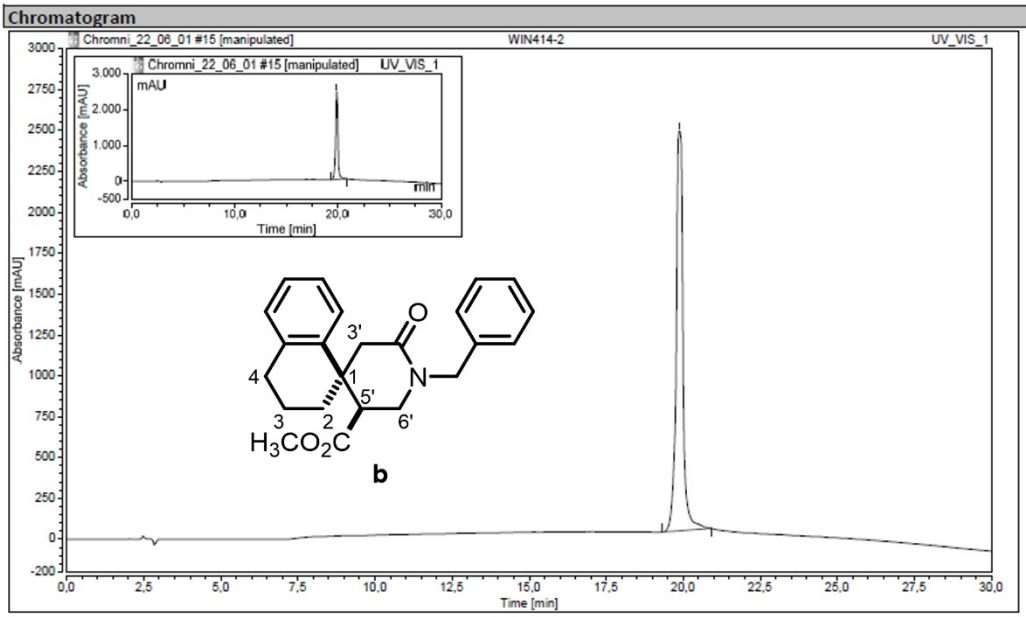
Methyl (1*SR*,5'*SR*)-1'-benzyl-2'-oxo-3,4-dihydro-2*H*-spiro(naphthalene-1,4'-piperidine)-5'-carboxylate (19b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN414-2**	*Run Time (min):*	**30,00**
Vial Number:	**GB3**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**02.Jun.22 00:22**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		19,883	631,869	2447,296	100,00	100,00	n.a.
Total:			**631,869**	**2447,296**	**100,00**	**100,00**	

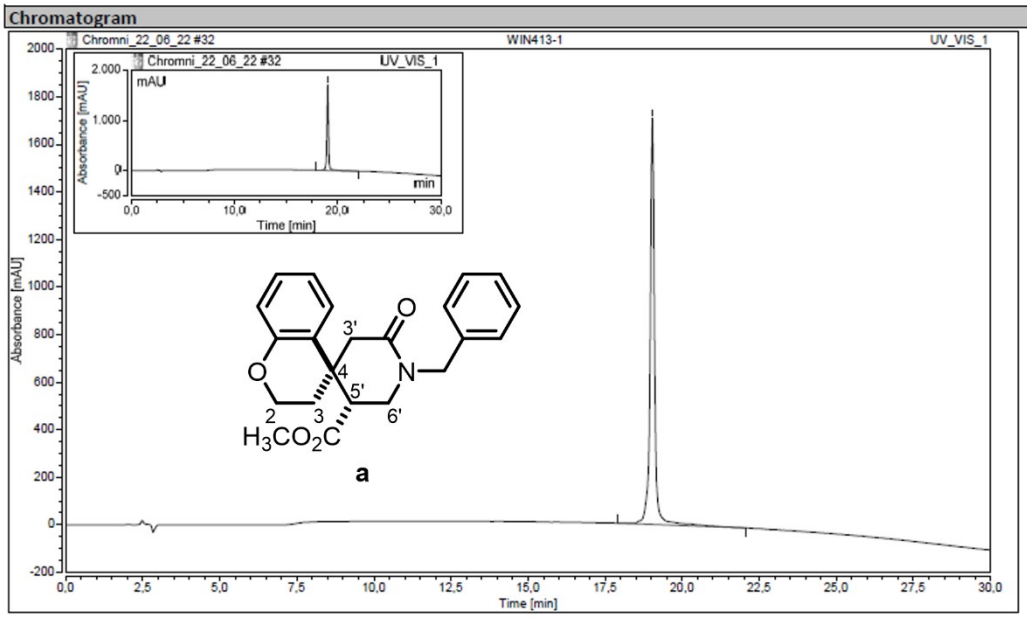
Methyl (4*RS*,5'*SR*)-1'-benzyl-2'-oxospiro(chromane-4,4'-piperidine)-5'-carboxylate (20a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN413-1**	*Run Time (min):*	**30,00**
Vial Number:	**GD2**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**23.Jun.22 11:38**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		19,028	289,079	1709,917	100,00	100,00	n.a.
Total:			**289,079**	**1709,917**	**100,00**	**100,00**	

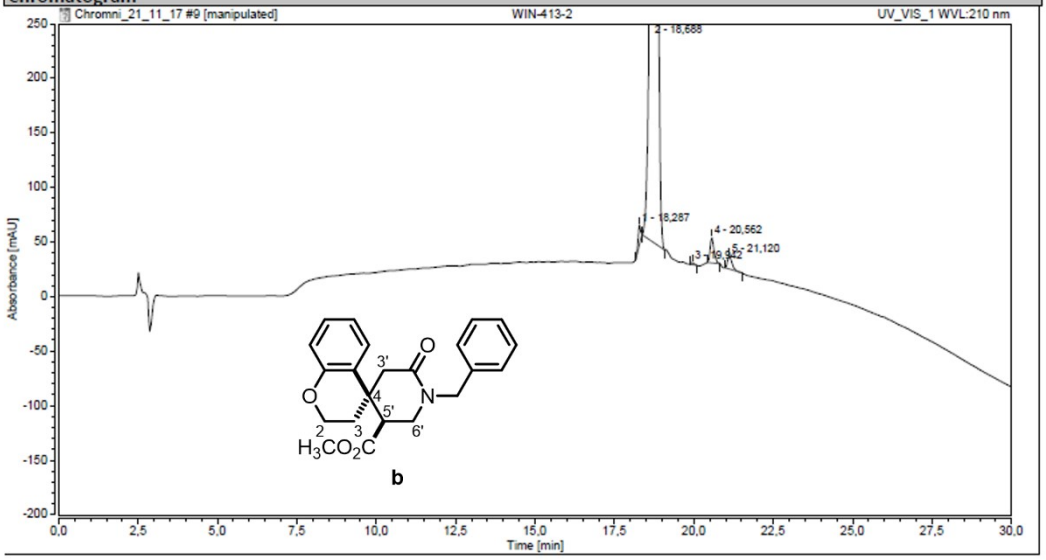
Methyl (4*RS*,5'*RS*)-1'-benzyl-2'-oxospiro(chromane-4,4'-piperidine)-5'-carboxylate (20b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN-413-2**	*Run Time (min):*	**30,00**
Vial Number:	**GA7**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**17.Nov.21 18:02**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		18,287	1,502	17,278	0,47	0,92	n.a.
2		18,688	309,512	1820,974	97,82	97,11	n.a.
3		19,942	0,213	1,865	0,07	0,10	n.a.
4		20,562	3,279	23,146	1,04	1,23	n.a.
5		21,120	1,896	11,923	0,60	0,64	n.a.
Total:			**316,402**	**1875,185**	**100,00**	**100,00**	

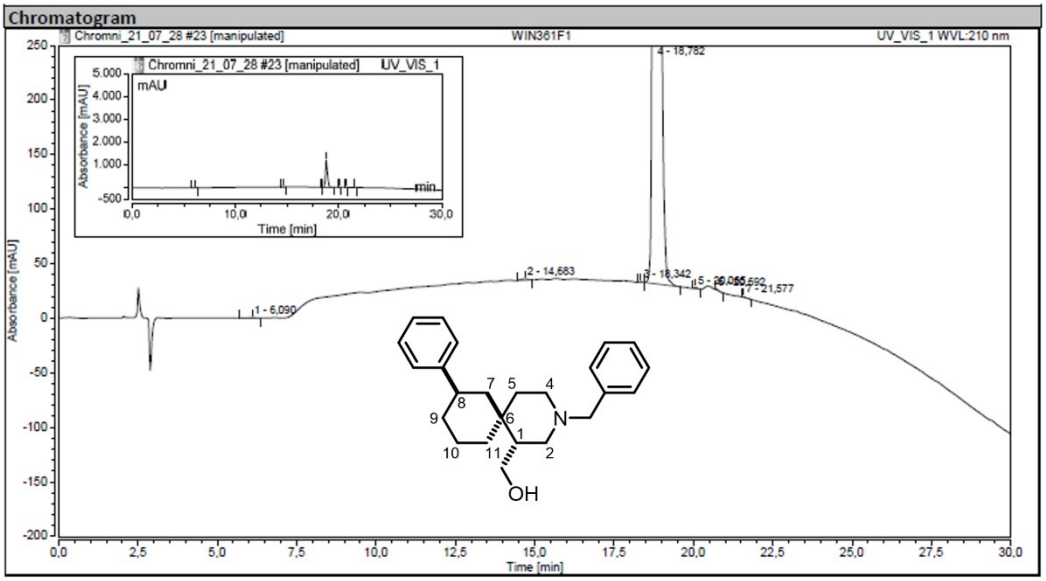
((1*RS*,6*SR*,8*RS*)-3-Benzyl-8-phenyl-3-azaspiro[5.5]undecan-1-yl)methanol (21a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN361F1**	*Run Time (min):*	**30,00**
Vial Number:	**GC4**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**29.Jul.21 02:38**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		6,090	0,138	0,394	0,05	0,03	n.a.
2		14,683	0,281	1,059	0,10	0,09	n.a.
3		18,342	0,081	0,848	0,03	0,07	n.a.
4		18,782	272,161	1192,168	99,73	99,64	n.a.
5		20,065	0,126	1,027	0,05	0,09	n.a.
6		20,692	0,058	0,410	0,02	0,03	n.a.
7		21,577	0,057	0,524	0,02	0,04	n.a.
Total:			**272,902**	**1196,429**	**100,00**	**100,00**	

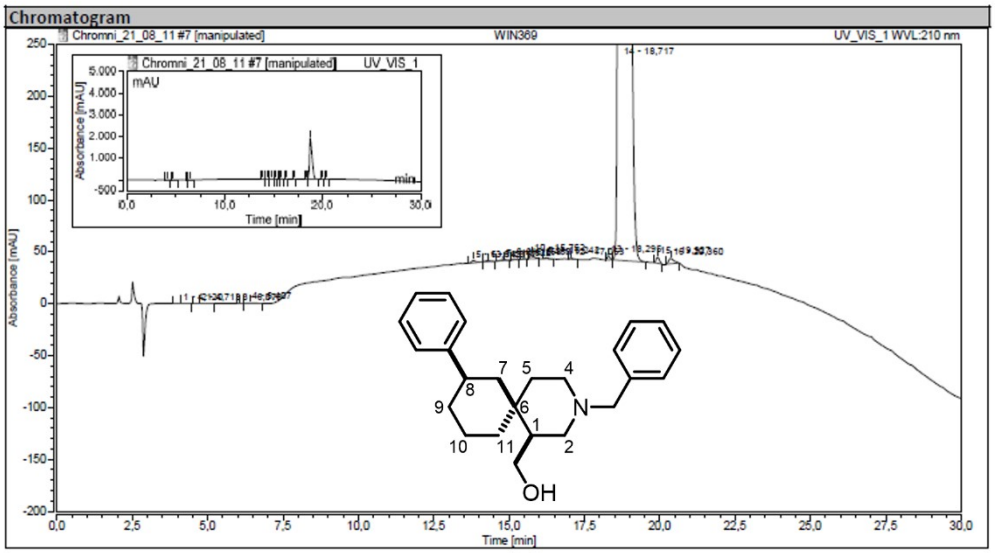
((1*RS*,6*RS*,8*SR*)-3-Benzyl-8-phenyl-3-azaspiro[5.5]undecan-1-yl)methanol (21b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN369**	*Run Time (min):*	**30,00**
Vial Number:	**GA5**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**11.Aug.21 15:39**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		4,120	0,092	0,296	0,02	0,02	n.a.
2		4,713	0,064	0,193	0,01	0,01	n.a.
3		6,078	0,007	0,066	0,00	0,00	n.a.
4		6,407	0,126	0,362	0,02	0,02	n.a.
5		13,812	0,351	2,232	0,06	0,12	n.a.
6		14,317	0,165	0,783	0,03	0,04	n.a.
7		14,822	0,234	1,154	0,04	0,06	n.a.
8		15,163	0,099	0,835	0,02	0,04	n.a.
9		15,480	0,080	0,908	0,01	0,05	n.a.
10		15,752	0,664	4,227	0,11	0,22	n.a.
11		16,242	0,136	1,000	0,02	0,05	n.a.
12		17,063	0,133	0,977	0,02	0,05	n.a.
13		18,295	0,399	3,852	0,07	0,20	n.a.
14		18,717	598,422	1894,142	99,28	98,55	n.a.
15		19,927	0,707	5,840	0,12	0,30	n.a.
16		20,360	1,059	5,185	0,18	0,27	n.a.
Total:			**602,737**	**1922,050**	**100,00**	**100,00**	

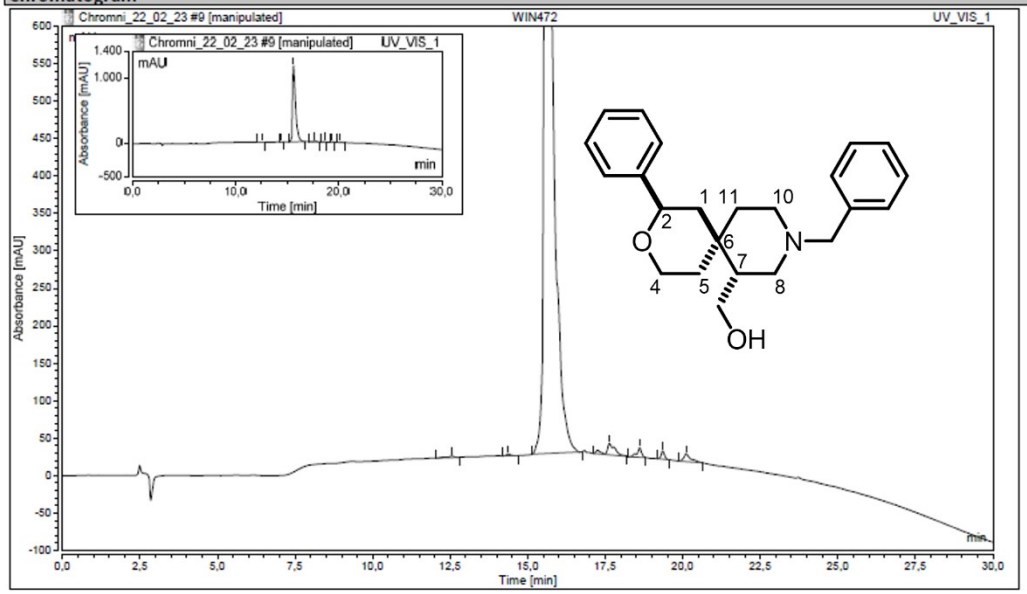
((2*RS*,6*SR*,7*RS*)-9-Benzyl-2-phenyl-3-oxa-9-azaspiro[5.5]undecan-7-yl)methanol (22a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN472**	*Run Time (min):*	**30,00**
Vial Number:	**GA7**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**23.Feb.22 20:59**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		12,548	0,560	2,234	0,14	0,18	n.a.
2		14,373	0,374	2,630	0,10	0,22	n.a.
3		15,600	374,069	1157,727	96,85	95,40	n.a.
4		17,637	5,024	15,503	1,30	1,28	n.a.
5		18,610	2,177	13,197	0,56	1,09	n.a.
6		19,352	1,357	11,514	0,35	0,95	n.a.
7		20,108	2,665	10,707	0,69	0,88	n.a.
Total:			**386,226**	**1213,512**	**100,00**	**100,00**	

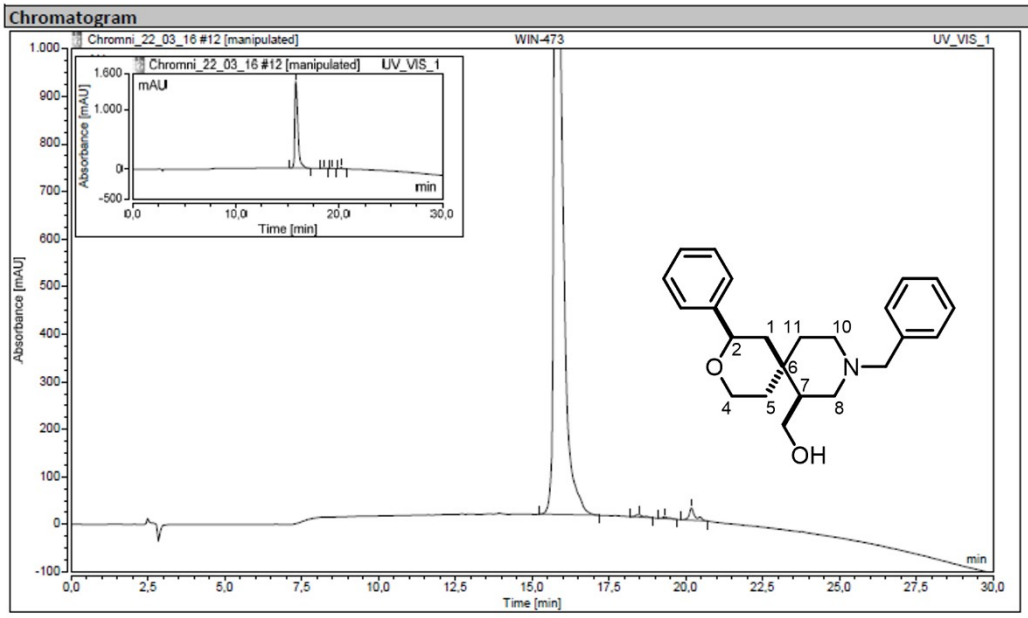
((2*RS*,6*SR*,7*SR*)-9-Benzyl-2-phenyl-3-oxa-9-azaspiro[5.5]undecan-7-yl)methanol (22b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN-473**	*Run Time (min):*	**30,00**
Vial Number:	**GB1**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**16.Mrz.22 22:34**	*Sample Weight:*	**1,0000**

Chromatogram

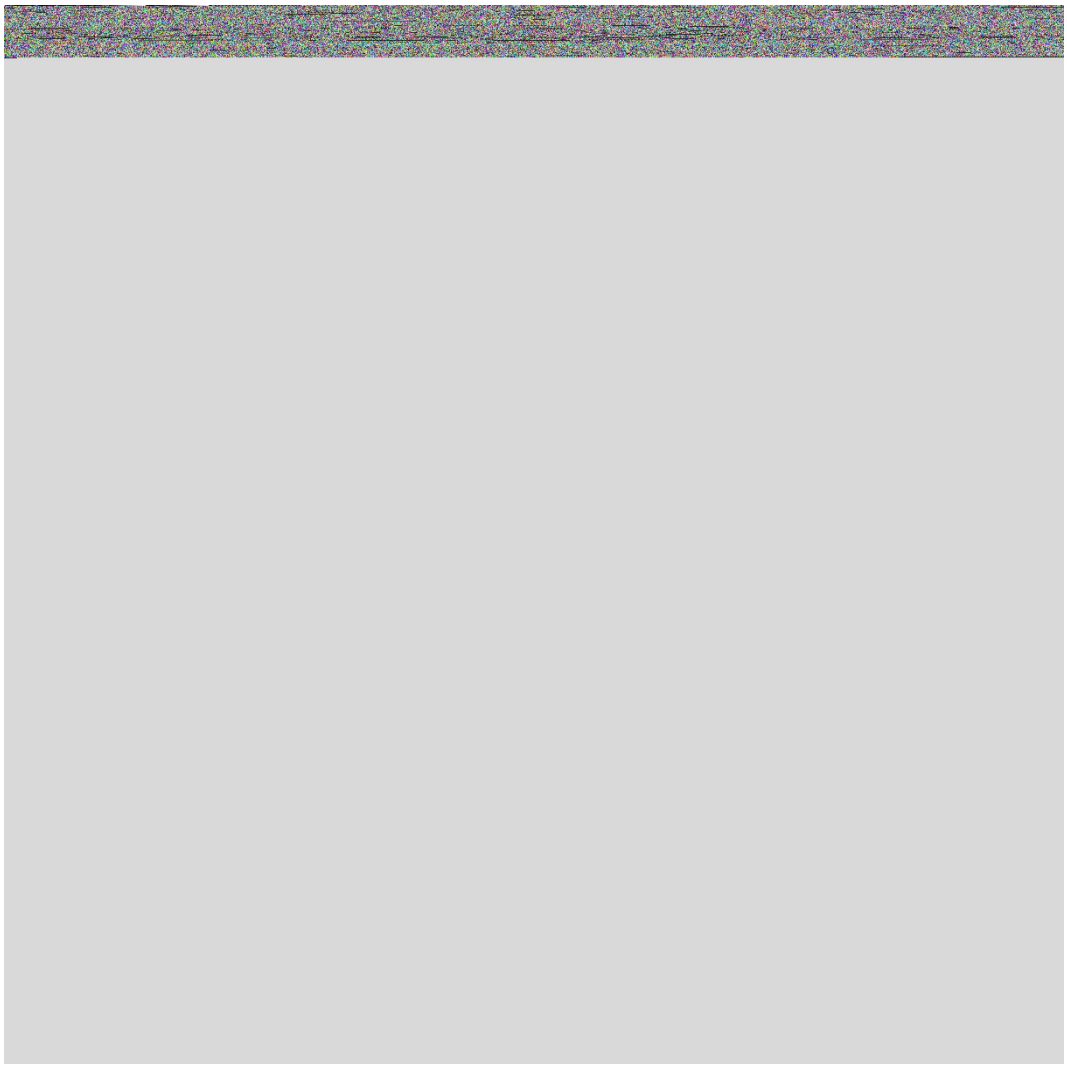


Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15,777	489,622	1458,521	98,35	97,63	n.a.
2		18,493	1,513	5,004	0,30	0,33	n.a.
3		19,307	0,820	4,033	0,16	0,27	n.a.
4		20,183	5,892	26,323	1,18	1,76	n.a.
Total:			**497,848**	**1493,882**	**100,00**	**100,00**	

((1*RS*,6*SR*)-3-Benzyl-14-oxa-3-azadispiro[5.1.5^{8}.3^{6}]hexadecan-1-yl)methanol (23a)

((1*RS*,6*RS*)-3-Benzyl-14-oxa-3-azadispiro[5.1.5^{8}.3^{6}]hexadecan-1-yl)methanol (23b)



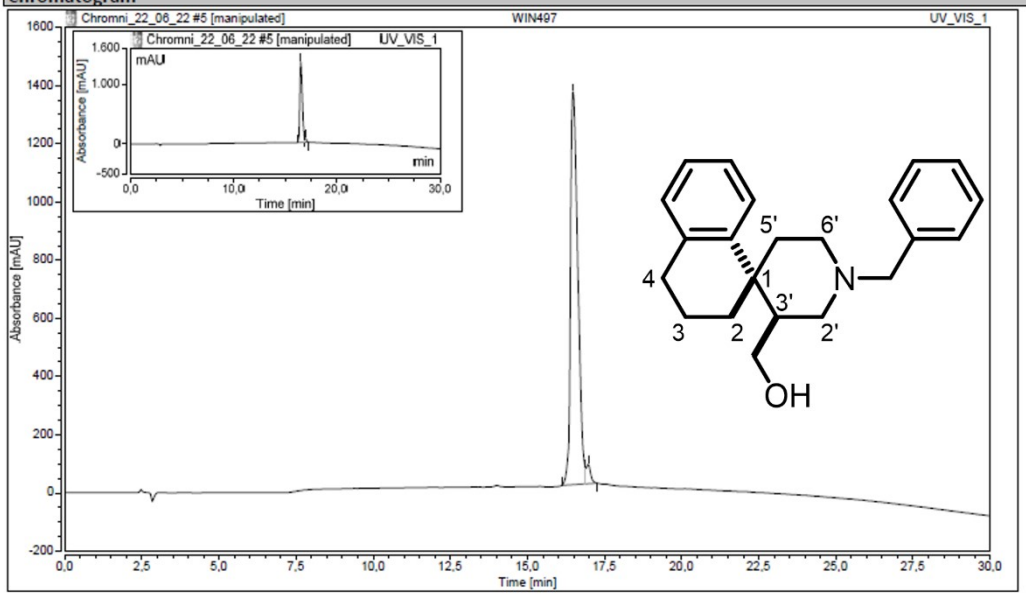
((1*RS*,3'*SR*)-1'-Benzyl-3,4-dihydrospiro[naphthalene-1(2*H*),4'-piperidin]-3'-yl)methanol (24a)

Chromatogram and Results

Injection Details

Injection Name:	**WIN497**	*Run Time (min):*	**30,00**
Vial Number:	**GA2**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**22.Jun.22 17:18**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		16,478	372,549	1350,366	96,94	95,28	n.a.
2		16,970	11,777	66,932	3,06	4,72	n.a.
Total:			**384,325**	**1417,297**	**100,00**	**100,00**	

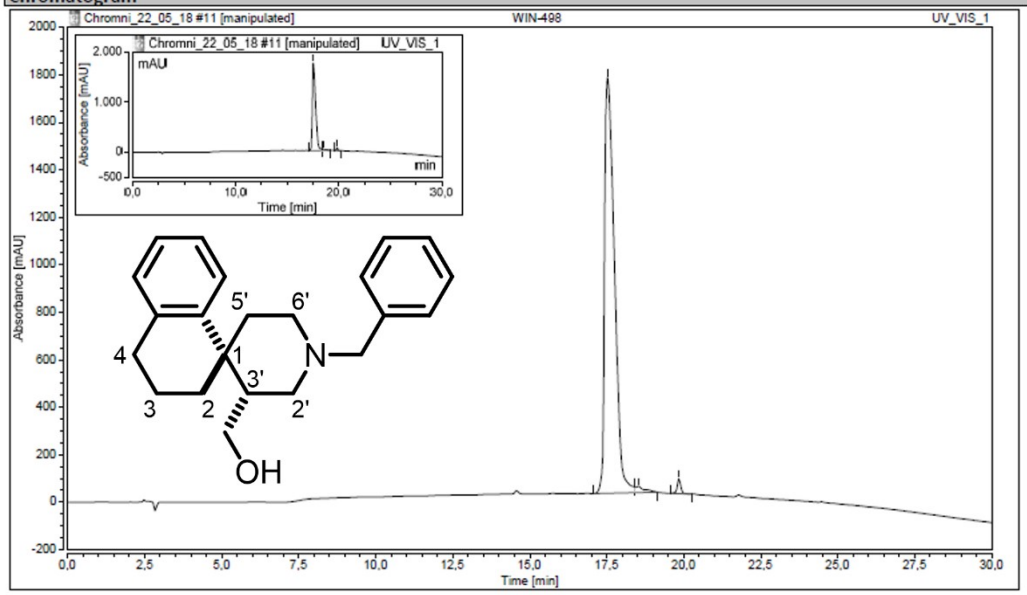
((1*RS*,3'*RS*)-1'-Benzyl-3,4-dihydrospiro[naphthalene-1(2*H*),4'-piperidin]-3'-yl)methanol (24b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN-498**	*Run Time (min):*	**30,00**
Vial Number:	**GA8**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**18.Mai.22 21:18**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		17,525	649,308	1750,289	97,32	95,06	n.a.
2		18,535	9,564	27,194	1,43	1,48	n.a.
3		19,842	8,309	63,834	1,25	3,47	n.a.
Total:			**667,181**	**1841,316**	**100,00**	**100,00**	

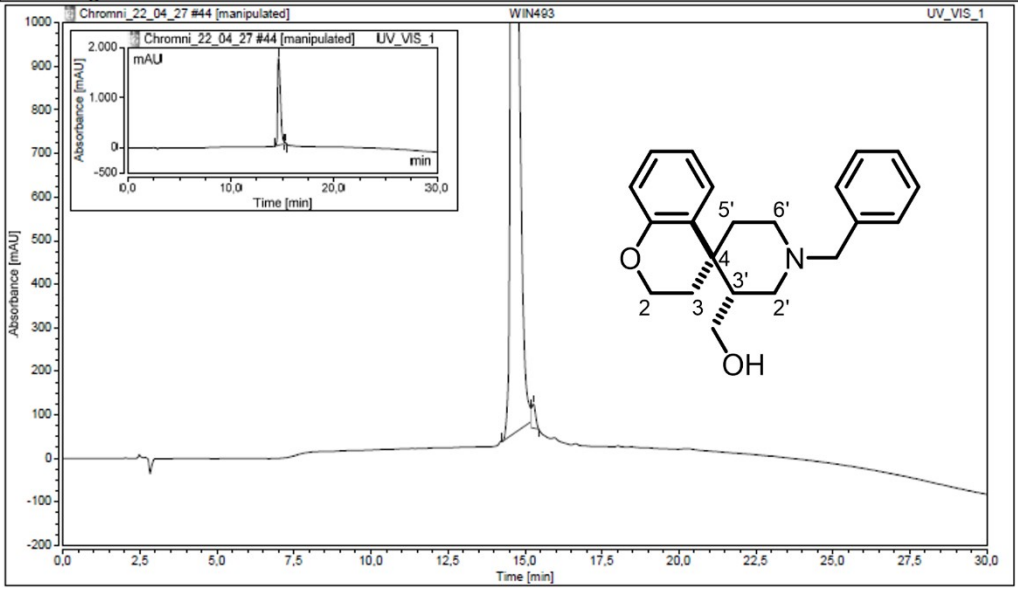
((3'*RS*,4*RS*)-1'-Benzylspiro[chromane-4,4'-piperidin]-3'-yl)methanol (25a)

Chromatogram and Results

Injection Details

Injection Name:	WIN493	*Run Time (min):*	30,00
Vial Number:	GE5	*Injection Volume:*	5,00
Injection Type:	Unknown	*Channel:*	UV_VIS_1
Calibration Level:		*Wavelength:*	210,0
Instrument Method:	Chromni	*Bandwidth:*	n.a.
Processing Method:	Chromni Processing Method	*Dilution Factor:*	1,0000
Injection Date/Time:	28.Apr.22 19:42	*Sample Weight:*	1,0000

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		14,602	557,031	1758,637	98,43	96,90	n.a.
2		15,275	8,911	56,314	1,57	3,10	n.a.
Total:			**565,941**	**1814,950**	**100,00**	**100,00**	

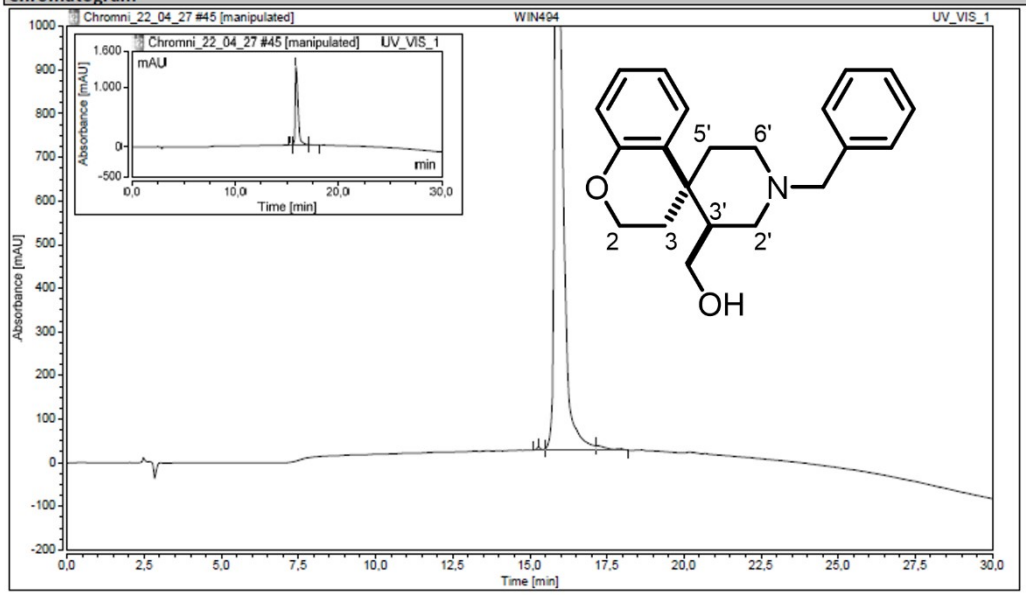
((3'*RS*,4*SR*)-1'-Benzylspiro[chromane-4,4'-piperidin]-3'-yl)methanol (25b)

Chromatogram and Results

Injection Details

Injection Name:	**WIN494**	*Run Time (min):*	**30,00**
Vial Number:	**GE6**	*Injection Volume:*	**5,00**
Injection Type:	**Unknown**	*Channel:*	**UV_VIS_1**
Calibration Level:		*Wavelength:*	**210,0**
Instrument Method:	**Chromni**	*Bandwidth:*	**n.a.**
Processing Method:	**Chromni Processing Method**	*Dilution Factor:*	**1,0000**
Injection Date/Time:	**28.Apr.22 20:22**	*Sample Weight:*	**1,0000**

Chromatogram



Integration Results

No.	Peak Name	Retention Time min	Area mAU*min	Height mAU	Relative Area %	Relative Height %	Amount n.a.
1		15,278	1,047	6,782	0,24	0,51	n.a.
2		15,873	431,511	1320,944	98,73	98,74	n.a.
3		17,130	4,508	10,118	1,03	0,76	n.a.
Total:			**437,066**	**1337,845**	**100,00**	**100,00**	