

Supporting Information

Chiral Phosphoric Acid Catalyzed Asymmetric C(sp³)-H Functionalization of Biomass-Derived 2,5-Dimethylfuran via Two Sequential Cope-Type Rearrangements

Lubin Xu,^{a§} Haohua Chen,^{c§} Jian Liu,^{a§} Lan Zhou,^a Qing Liu,^e Yu Lan,^{*cd} Jian Xiao,^{*ab}

^a College of Chemistry and Pharmaceutical Sciences, Qingdao Agricultural University, Qingdao 266109, China

^b College of Marine Science and Engineering, Qingdao Agricultural University, Qingdao 266109, China

^c School of Chemistry and Chemical Engineering, Chongqing University, Chongqing 400030, China

^d College of Chemistry and Molecular Engineering, Zhengzhou University, Zhengzhou 450001, P. R. China

^e College of Chemical and Environmental Engineering, Shandong University of Science and Technology, Qingdao 266590, China

[§]These authors contributed equally.

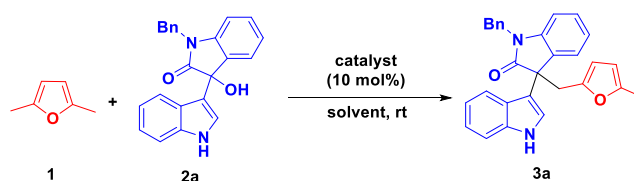
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1. General Information

^1H and ^{13}C NMR spectra were measured respectively at 500 and 125 MHz, respectively. The solvent used for NMR spectroscopy was CDCl_3 , using tetramethylsilane as the internal reference. HRMS (ESI) was determined by a micr OTOF-QII HRMS/MS instrument (Bruker). The chiral columns used for the determination of ee by chiral HPLC were Chiralpak IF and AS-H columns. Optical rotation values were measured with instruments operating at $\lambda = 589\text{ nm}$, corresponding to the sodium D line at the temperatures indicated. Analytic grade solvents for the chromatography and commercially available reagents were used as received. Substrates **2** were synthesized according to the literature methods¹.

2. Optimization of the reaction conditions ^a

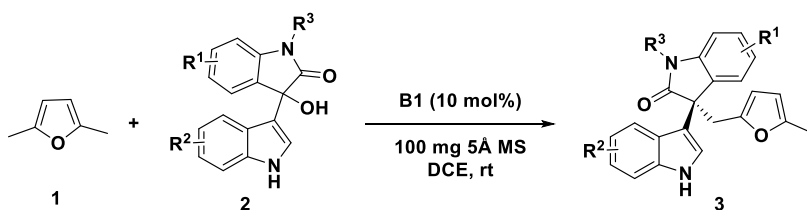


entry	acid (20 mol%)	solvent	time	yield(%) ^b
1	2,4-Dinitrobenzoic acid	DCE	48 h	trace
2	Benzoic acid	DCE	24 h	trace
3	PA	DCE	48 h	75
4	CSA	DCE	48 h	71
5	TFA	DCE	72 h	31
6	TsOH	DCE	48 h	23
7	TfOH	DCE	48 h	28
8	$\text{Sc}(\text{OTf})_3$	DCE	24 h	12
9	InBr_3	DCE	36 h	trace
10	PA	DCM	24 h	56
11	PA	CHCl_3	24 h	65
12	PA	THF	48 h	trace
13	PA	Toluene	24 h	trace
14	PA	CH_3CN	24 h	n.r
15	PA	Dioxane	48 h	trace
16	PA (5 mol%)	DCE	72 h	12
17	PA (10 mol%)	DCE	48 h	52
18	PA (30 mol%)	DCE	10 h	41

^a Reaction were conducted with **1a** (0.1 mmol), **2a** (0.3 mmol), and catalyst (20 mol%) in 2 mL of solvent. ^b Isolated yield after column chromatography. PA = (+/-)-1,1'-Binaphthyl-2,2'-diyl Hydrogenphosphate ; DCM = Dichloromethane; DCE = Dichloroethane; THF = Tetrahydrofuran.

¹ Wang, X.-X.; Liu, J.; Xu, L.-B.; Hao, Z.-H.; Wang, L.; Xiao, J. *RSC. Adv.* **2015**, 5, 101713.

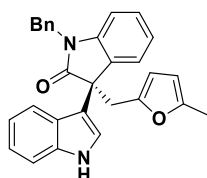
3. General Procedure for Synthesis of Products 3



To a 25 mL pressure tube equipped with a magnetic stirrer bar were added DCE (2 mL), indoly alcohol **1** (0.1 mmol), 2,5-dimethylfuran **2** (0.5 mmol), catalyst **B1** (0.01mmol) and 5 Å MS (100 mg). The mixture was then stirred at room temperature. Reaction was monitored by TLC with silica gel-coated plates. The solvent was removed *in vacuo*. The residue was then purified by column chromatography on silica gel to afford the desired product **3**.

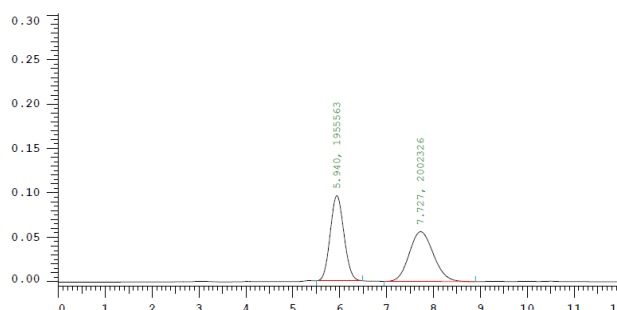
4. Characterization Data of All Products

(R)-1-benzyl-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3a)

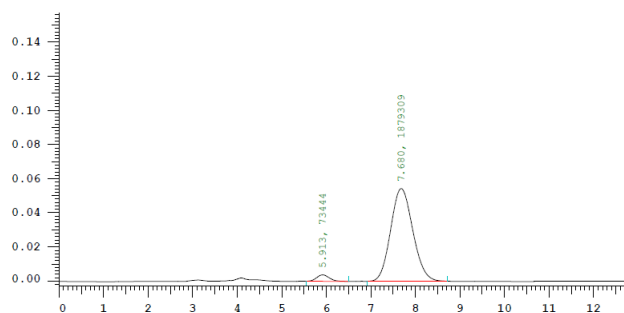


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 89%; white solid; $[\alpha]_D^{20} = +33.6$ ($c = 0.26$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 5.913$ min (minor), $t_R = 7.680$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.16 (s, 1H), 7.31 (d, $J = 8.2$ Hz, 1H), 7.22 (t, $J = 8.7$ Hz, 5H), 7.18 – 7.10 (m, 2H), 7.10 – 7.06 (m, 2H), 7.01 (t, $J = 7.5$ Hz, 1H), 6.92 (t, $J = 7.5$ Hz, 1H), 6.66 (d, $J = 7.8$ Hz, 1H), 5.68 (s, 1H), 5.58 (d, $J = 2.5$ Hz, 1H), 4.94 (d, $J = 15.7$ Hz, 1H), 4.80 (d, $J = 15.8$ Hz, 1H), 3.92 (t, $J = 11.9$ Hz, 1H), 3.65 (d, $J = 14.4$ Hz, 1H), 2.04 (s, 3H); **^{13}C NMR** (125 MHz, CDCl_3) δ 178.05, 150.70, 148.78, 143.09, 136.91, 135.83, 132.11, 128.59, 128.09, 127.36, 127.27, 125.48, 124.90, 122.94, 122.38, 122.26, 120.78, 119.74, 115.24, 111.30, 109.02, 108.69, 105.96, 52.96, 43.98, 35.16, 13.40; **HRMS** (ESI) calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 455.1730, found 455.1726;

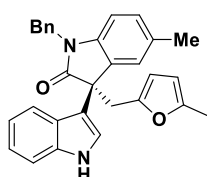


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	5.940	1955563	95812	49.409
2	7.727	2002326	56005	50.591
Total		3957889	151817	100.00



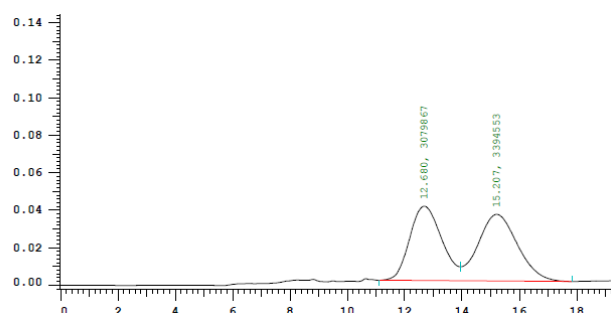
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	5.913	73444	3779	3.761
2	7.680	1879309	54291	96.239
Total		1952753	58070	100.00

(R)-1-benzyl-3-(1H-indol-3-yl)-5-methyl-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3b)

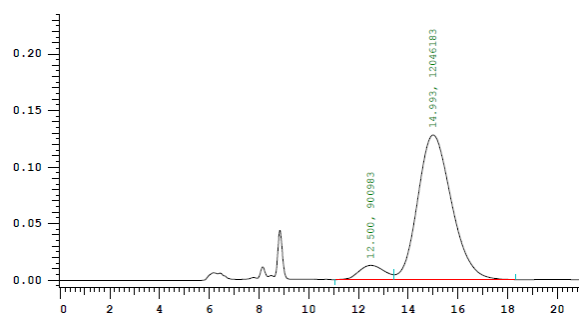


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 62%; white solid; $[\alpha]_D^{20} = +9.7$ ($c = 0.23$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 12.500$ min (minor), $t_R = 14.993$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.23 (s, 1H), 7.23 (d, $J = 2.6$ Hz, 4H), 7.19 (d, $J = 7.3$ Hz, 1H), 7.15 (t, $J = 7.7$ Hz, 1H), 7.09 (dd, $J = 10.4, 6.7$ Hz, 2H), 6.99 (t, $J = 7.5$ Hz, 1H), 6.93 – 6.84 (m, 2H), 6.80 (q, $J = 7.2$ Hz, 1H), 6.66 (d, $J = 7.8$ Hz, 1H), 5.68 (s, 1H), 5.58 (t, $J = 4.3$ Hz, 1H), 4.93 (d, $J = 15.7$ Hz, 1H), 4.83 (d, $J = 15.8$ Hz, 1H), 3.93 (d, $J = 14.4$ Hz, 1H), 3.65 (d, $J = 14.3$ Hz, 1H), 2.34 (s, 3H), 2.04 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.34, 150.71, 148.77, 143.09, 136.41, 135.83, 132.30, 128.60, 128.06, 127.38, 127.30, 124.88, 122.88, 122.66, 122.48, 120.49, 119.83, 118.12, 115.37, 108.99, 108.71, 105.97, 52.99, 44.03, 35.18, 16.47, 13.41. **HRMS** (ESI) calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 469.1886, found 469.1890;

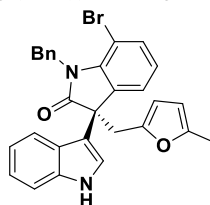


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	12.680	3079867	39640	47.570
2	15.207	3394553	35488	52.430
Total		6474420	75128	100.00



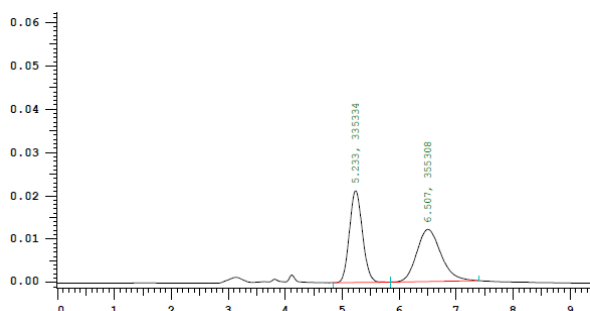
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	12.500	900983	12627	6.959
2	14.993	12046183	127933	93.041
Total		12947166	140560	100.00

(R)-1-benzyl-7-bromo-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3c)

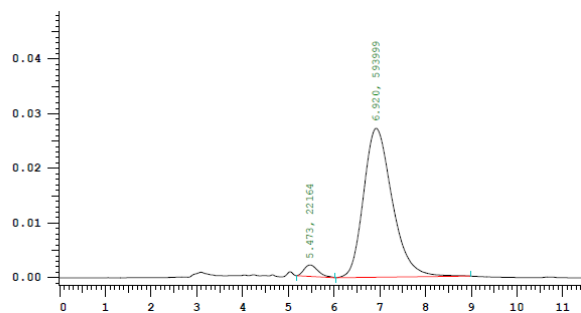


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 65%; white solid; $[\alpha]_D^{20} = +53.9$ ($c = 0.32$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 1.0 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 5.233$ min (minor), $t_R = 6.500$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.14 (s, 1H), 7.32 (d, $J = 8.2$ Hz, 1H), 7.22 (dd, $J = 7.6, 5.4$ Hz, 6H), 7.18 – 7.11 (m, 2H), 7.10 – 7.05 (m, 2H), 7.01 (t, $J = 7.5$ Hz, 1H), 6.93 (t, $J = 7.6$ Hz, 1H), 6.66 (d, $J = 7.8$ Hz, 1H), 5.68 (d, $J = 2.1$ Hz, 1H), 5.58 (d, $J = 2.9$ Hz, 1H), 4.94 (d, $J = 15.8$ Hz, 1H), 4.80 (d, $J = 15.8$ Hz, 1H), 3.96 – 3.92 (m, 1H), 3.65 (d, $J = 14.4$ Hz, 1H), 2.04 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.82, 151.00, 148.26, 140.70, 137.60, 136.89, 135.48, 134.09, 128.37, 126.78, 126.43, 125.20, 124.20, 123.66, 123.06, 122.36, 120.56, 119.87, 114.73, 111.43, 109.09, 106.11, 102.14, 52.78, 44.81, 35.51, 13.45. **HRMS** (ESI) calcd for $\text{C}_{29}\text{H}_{23}\text{BrN}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 533.0835, found 533.0832.

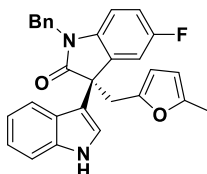


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	5.233	335334	21158	48.554
2	6.507	335308	12006	51.446
Total		690642	33164	100.00



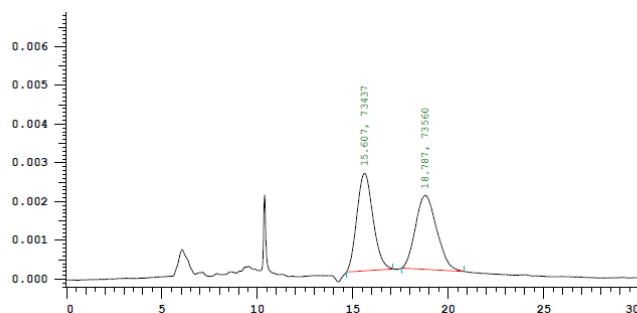
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	5.473	22164	1041	3.597
2	6.920	593999	13610	96.403
Total		616163	14651	100.00

(R)-1-benzyl-5-fluoro-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3d)

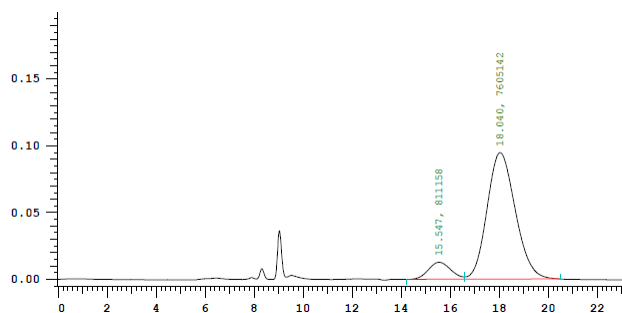


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 63%; white solid; $[\alpha]_D^{20} = +57.0$ ($c = 0.26$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 75/25, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 15.547$ min (minor), $t_R = 18.040$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.30 (s, 1H), 7.32 (d, $J = 8.3$ Hz, 1H), 7.24 (s, 3H), 7.17 (s, 1H), 7.15 – 7.10 (m, 2H), 7.06 (d, $J = 15.3$ Hz, 2H), 6.92 (d, $J = 8.2$ Hz, 2H), 6.85 (t, $J = 8.7$ Hz, 1H), 6.56 (dd, $J = 8.4, 4.0$ Hz, 1H), 5.71 (s, 1H), 5.67 (s, 1H), 4.95 – 4.89 (m, 1H), 4.81 (dd, $J = 15.7, 5.6$ Hz, 1H), 3.90 (d, $J = 14.3$ Hz, 1H), 3.62 (d, $J = 14.5$ Hz, 1H), 2.05 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 177.92, 150.96, 148.34, 138.95, 136.89, 135.49, 128.68, 127.52, 127.26, 125.29, 122.95, 122.38, 120.39, 119.85, 114.53, 114.45, 114.26, 113.03, 112.83, 111.44, 109.50, 109.43, 108.97, 106.01, 77.29, 77.04, 76.78, 53.42, 44.16, 35.08, 13.39. **HRMS** (ESI) calcd for $\text{C}_{29}\text{H}_{23}\text{FN}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 473.1636, found 473.1633.

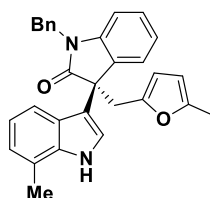


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	15.607	73437	1258	49.958
2	18.787	73560	953	50.042
Total		146997	2211	100.00



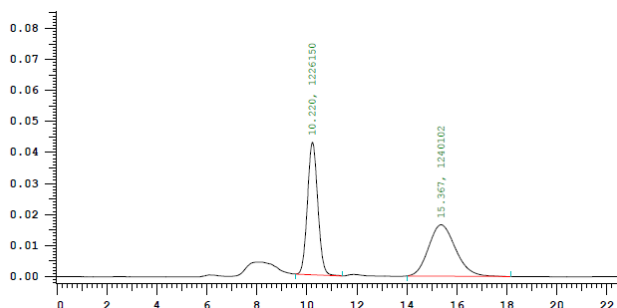
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	15.547	811158	12785	9.638
2	18.040	7605142	94718	90.362
Total		8416300	107503	100.00

(R)-1-benzyl-3-(7-methyl-1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3e)

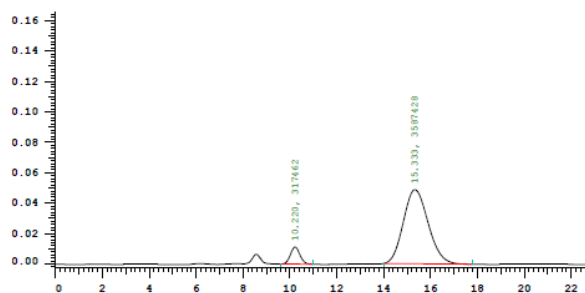


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 53%; white solid; $[\alpha]_D^{20} = +5.8$ ($c = 0.28$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 10.220$ min (minor), $t_R = 15.333$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.23 (s, 1H), 7.23 (d, $J = 2.6$ Hz, 4H), 7.19 (d, $J = 7.3$ Hz, 1H), 7.15 (t, $J = 7.7$ Hz, 1H), 7.09 (dd, $J = 10.4, 6.7$ Hz, 2H), 6.99 (t, $J = 7.5$ Hz, 1H), 6.93 – 6.84 (m, 2H), 6.80 (q, $J = 7.2$ Hz, 1H), 6.66 (d, $J = 7.8$ Hz, 1H), 5.68 (s, 1H), 5.58 (t, $J = 4.3$ Hz, 1H), 4.93 (d, $J = 15.7$ Hz, 1H), 4.83 (d, $J = 15.8$ Hz, 1H), 3.93 (d, $J = 14.4$ Hz, 1H), 3.65 (d, $J = 14.3$ Hz, 1H), 2.34 (s, 3H), 2.04 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.34, 150.71, 148.77, 143.09, 136.41, 135.83, 132.30, 128.60, 128.06, 127.38, 127.30, 124.88, 122.88, 122.66, 122.48, 120.49, 119.83, 118.12, 115.37, 108.99, 108.71, 105.97, 52.99, 44.03, 35.18, 16.47, 13.41. **HRMS** (ESI) calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 469.1886, found 469.1886.

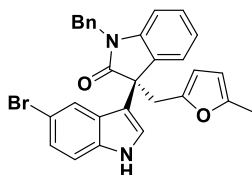


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	10.220	1226150	42708	49.717
2	15.367	1240102	16560	50.283
Total		2466252	59268	100.00



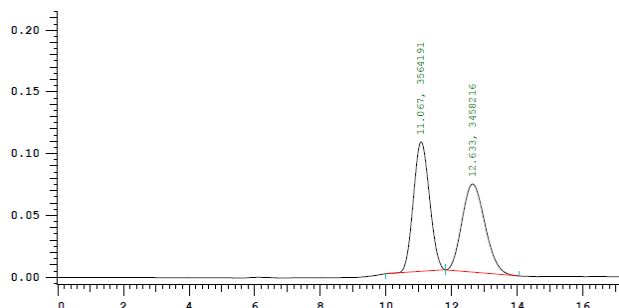
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	10.220	317462	11183	8.130
2	15.333	3587428	48688	91.870
Total		3904890	59871	100.00

(R)-1-benzyl-3-(5-bromo-1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3f)

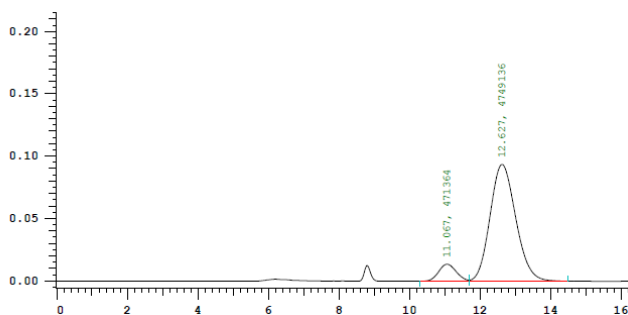


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 94% (24.0 mg); white solid; $[\alpha]_D^{20} = +65.4$ (c = 0.37, CHCl₃). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 0.5 mL/min, T = 25°C, 250 nm, t_R = 11.067 min (minor), t_R = 12.627 min (major).

¹H NMR (500 MHz, CDCl₃) δ 8.42 (s, 1H), 7.31 (s, 1H), 7.29 – 7.26 (m, 2H), 7.25 – 7.23 (m, 1H), 7.18 (tt, J = 8.7, 2.8 Hz, 4H), 7.12 – 7.10 (m, 2H), 7.09 (s, 1H), 7.03 (t, J = 7.3 Hz, 1H), 6.67 (d, J = 7.8 Hz, 1H), 5.69 (d, J = 2.1 Hz, 1H), 5.58 (d, J = 3.0 Hz, 1H), 4.91 (d, J = 15.8 Hz, 1H), 4.85 (d, J = 15.8 Hz, 1H), 3.85 (d, J = 14.4 Hz, 1H), 3.59 (d, J = 14.4 Hz, 1H), 2.05 (s, 3H). **¹³C NMR** (125 MHz, CDCl₃) δ 178.07, 150.82, 148.45, 143.00, 135.63, 135.52, 131.62, 128.78, 128.38, 127.43, 127.14, 127.06, 125.20, 124.83, 124.26, 123.20, 122.59, 114.74, 113.14, 112.76, 109.25, 108.81, 105.98, 77.28, 77.03, 76.78, 52.79, 44.05, 35.21, 13.40. **HRMS** (ESI) calcd for C₂₉H₂₃BrN₂NaO₂ [M+Na]⁺ 533.0835, found 533.0829.

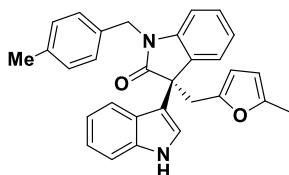


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	11.067	3564191	104631	50.755
2	12.633	3458216	71217	49.245
Total		7022407	175848	100.00



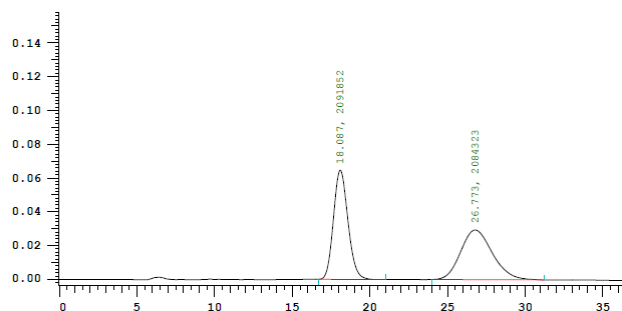
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	11.067	471364	13618	9.029
2	12.627	4749136	93628	90.971
Total		5220500	107246	100.00

(R)-3-(1H-indol-3-yl)-1-(4-methylbenzyl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3g)

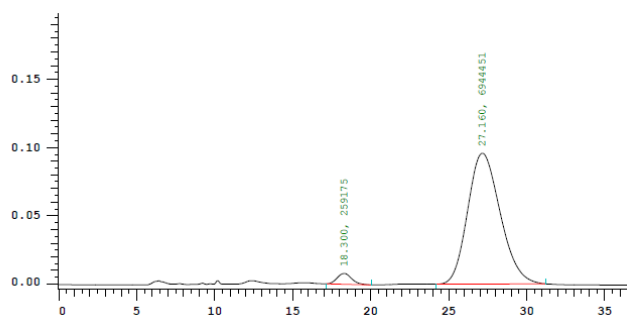


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 80%; white solid; $[\alpha]_D^{20} = +34.1$ ($c = 0.38$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 83/17, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 18.273$ min (minor), $t_R = 27.153$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.39 (s, 1H), 7.33 (d, $J = 8.4$ Hz, 1H), 7.19 – 7.08 (m, 5H), 7.04 (d, $J = 7.9$ Hz, 2H), 6.99 (t, $J = 7.4$ Hz, 3H), 6.90 (t, $J = 7.6$ Hz, 1H), 6.67 (d, $J = 7.8$ Hz, 1H), 5.68 (d, $J = 1.9$ Hz, 1H), 5.57 (d, $J = 2.9$ Hz, 1H), 4.89 (d, $J = 15.7$ Hz, 1H), 4.79 (d, $J = 15.6$ Hz, 1H), 3.90 (d, $J = 14.4$ Hz, 1H), 3.62 (d, $J = 14.4$ Hz, 1H), 2.31 (s, 3H), 2.05 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.24, 150.68, 148.78, 143.14, 136.99, 136.90, 132.76, 132.20, 129.27, 128.06, 127.25, 125.50, 124.85, 123.10, 122.37, 122.16, 120.62, 119.64, 115.01, 111.36, 109.07, 108.64, 105.94, 52.94, 43.80, 35.14, 21.13, 13.39. **HRMS** (ESI) calcd for $\text{C}_{30}\text{H}_{26}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 469.1886, found 469.1883.

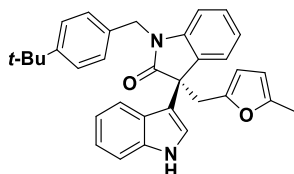


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	18.087	2091852	32272	50.090
2	26.773	2084323	14682	49.910
Total		4176175	46954	100.00



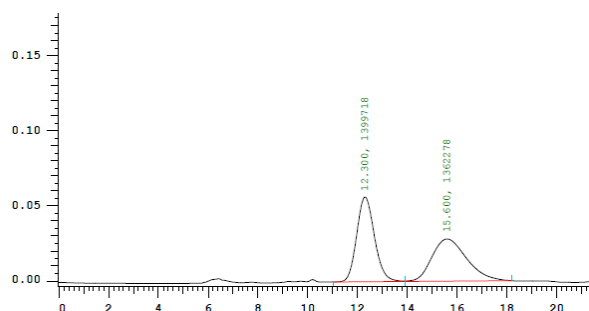
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	18.300	259175	3989	3.598
2	27.160	6944451	47858	96.402
Total		7203626	51847	100.00

(R)-1-(4-(tert-butyl)benzyl)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3h)



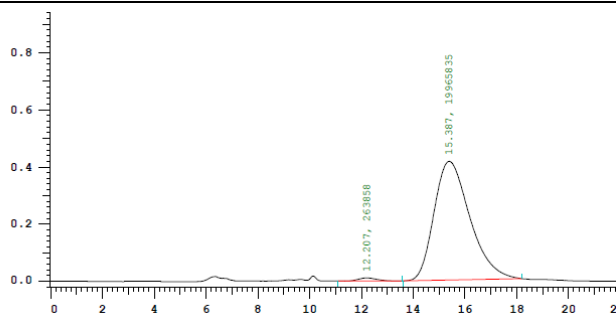
The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 84%; white solid; $[\alpha]_D^{20} = +26.7$ ($c = 0.21$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 83/17, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 12.207$ min (minor), $t_R = 15.387$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.39 (s, 1H), 7.33 (d, $J = 8.1$ Hz, 1H), 7.25 (s, 1H), 7.24 (s, 1H), 7.18 (ddd, $J = 7.7, 4.1, 1.7$ Hz, 2H), 7.15 – 7.08 (m, 3H), 7.05 (d, $J = 8.2$ Hz, 2H), 7.00 (t, $J = 7.5$ Hz, 1H), 6.89 (t, $J = 7.6$ Hz, 1H), 6.73 (d, $J = 7.9$ Hz, 1H), 5.67 (d, $J = 2.0$ Hz, 1H), 5.57 (d, $J = 2.9$ Hz, 1H), 4.89 (d, $J = 15.6$ Hz, 1H), 4.80 (d, $J = 15.7$ Hz, 1H), 3.89 (d, $J = 14.4$ Hz, 1H), 3.62 (d, $J = 14.4$ Hz, 1H), 2.03 (s, 3H), 1.29 (s, 9H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.23, 150.65, 150.23, 148.79, 143.23, 136.90, 132.79, 132.23, 128.05, 127.06, 125.51, 125.48, 124.85, 123.09, 122.35, 122.15, 120.65, 119.64, 115.02, 111.35, 109.03, 108.63, 105.94, 52.91, 43.67, 35.15, 34.47, 31.35, 26.94, 13.40. **HRMS** (ESI) calcd for $\text{C}_{33}\text{H}_{32}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 511.2356, found 511.2356.



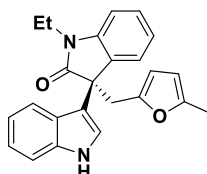
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	12.300	1399718	28169	50.678
2	15.600	1362278	14007	49.332

Total	2761996	42176	100.00
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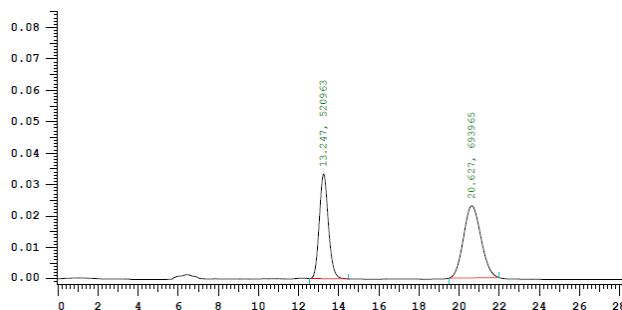
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	12.207	263858	5478	1.304
2	15.387	19965835	207604	98.696
Total		20229693	213082	100.00

(R)-1-ethyl-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3i)

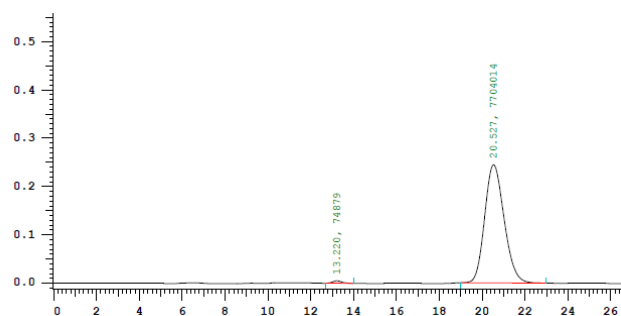


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 94%; white solid; $[\alpha]_D^{20} = +28.3$ ($c = 0.30$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 83/17, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 13.220$ min (minor), $t_R = 20.527$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.23 (s, 1H), 7.28 (d, $J = 6.9$ Hz, 1H), 7.20 – 7.13 (m, 3H), 7.08 (t, $J = 7.5$ Hz, 1H), 7.01 (t, $J = 7.5$ Hz, 1H), 6.92 (t, $J = 7.6$ Hz, 1H), 6.83 (d, $J = 7.8$ Hz, 1H), 5.63 (s, 1H), 5.55 (d, $J = 2.8$ Hz, 1H), 3.82 (td, $J = 14.4, 7.3$ Hz, 2H), 3.63 (dt, $J = 14.1, 7.1$ Hz, 1H), 3.57 (d, $J = 14.4$ Hz, 1H), 2.04 (s, 3H), 1.14 (t, $J = 7.2$ Hz, 3H) **^{13}C NMR** (125 MHz, CDCl_3) δ 177.64, 150.55, 148.78, 142.96, 136.89, 132.48, 128.06, 125.52, 124.99, 122.91, 122.14, 122.13, 120.49, 119.64, 114.94, 111.31, 108.36, 107.88, 105.80, 52.77, 35.36, 34.71, 13.36, 12.42. **HRMS** (ESI) calcd for $\text{C}_{24}\text{H}_{22}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 393.1573, found 393.1572.

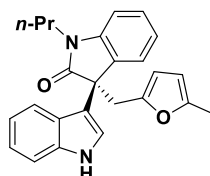


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	13.247	520963	16660	42.880
2	20.627	693965	11483	57.120
Total		10801984	28143	100.00



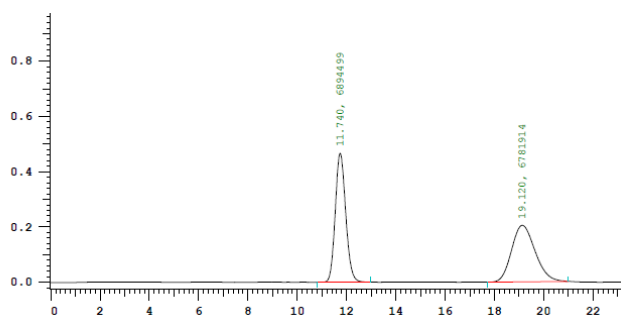
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	13.220	74879	2552	0.963
2	20.527	7704014	122082	99.037
Total		7778893	124634	100.00

(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-1-propylindolin-2-one(3j)



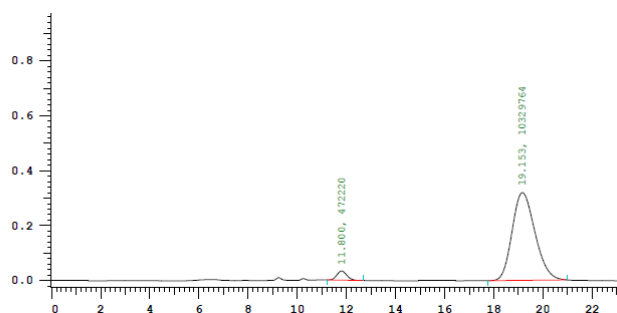
The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 83%; white solid; $[\alpha]_D^{20} = +20.3$ ($c = 0.40$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 83/17, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 11.800$ min (minor), $t_R = 19.153$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.17 (s, 1H), 7.26 (dd, $J = 12.0, 6.2$ Hz, 2H), 7.22 (d, $J = 8.1$ Hz, 1H), 7.19 – 7.14 (m, 2H), 7.09 (t, $J = 7.6$ Hz, 1H), 7.00 (dd, $J = 16.6, 9.1$ Hz, 1H), 6.93 (t, $J = 7.6$ Hz, 1H), 6.82 (d, $J = 7.8$ Hz, 1H), 5.63 (s, 1H), 5.55 (d, $J = 2.9$ Hz, 1H), 3.84 (d, $J = 14.4$ Hz, 1H), 3.72 – 3.63 (m, 1H), 3.59 (d, $J = 14.4$ Hz, 1H), 3.54 (dd, $J = 14.2, 7.5$ Hz, 1H), 2.04 (s, 3H), 1.62 – 1.56 (m, 2H), 0.88 (t, $J = 7.4$ Hz, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 177.88, 150.54, 148.82, 143.50, 136.89, 132.28, 128.04, 125.53, 124.98, 122.90, 122.15, 122.06, 120.65, 119.66, 115.12, 111.27, 108.36, 108.06, 105.83, 52.76, 41.81, 35.32, 20.76, 13.35, 11.48. **HRMS** (ESI) calcd for $\text{C}_{25}\text{H}_{24}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 407.1730, found 407.1731.



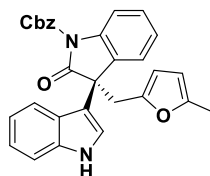
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	11.740	6894499	233436	50.412
2	19.120	6781914	102287	49.588

Total	13676413	335723	100.00
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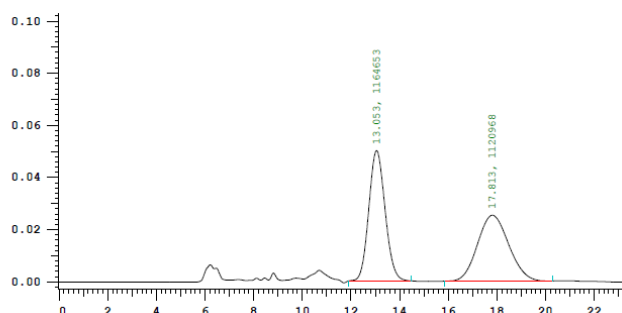
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	11.800	472220	16748	4.372
2	19.153	10329764	159815	95.628
Total		10801984	176563	100.00

(R)-benzyl-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-2-oxindoline-1-carboxylate(3k)

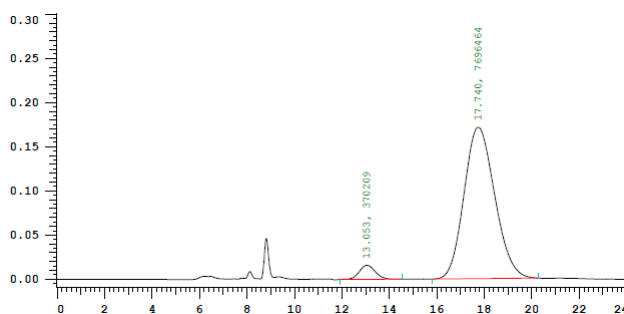


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 77%; white solid; $[\alpha]_D^{20} = +27.6$ ($c = 0.33$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 13.053$ min (minor), $t_R = 17.740$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.23 (s, 1H), 7.36 (d, $J = 8.0$ Hz, 1H), 7.26 (dd, $J = 8.6, 6.2$ Hz, 3H), 7.21 – 7.16 (m, 4H), 7.13 – 7.10 (m, 2H), 7.00 – 6.93 (m, 3H), 6.90 (t, $J = 7.7$ Hz, 1H), 5.74 (d, $J = 2.2$ Hz, 1H), 5.62 (d, $J = 2.9$ Hz, 1H), 5.32 (s, 2H), 3.95 (d, $J = 14.4$ Hz, 1H), 3.60 (d, $J = 14.4$ Hz, 1H), 2.07 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.00, 150.69, 148.78, 143.10, 136.91, 135.83, 132.08, 128.58, 128.09, 127.35, 127.27, 125.49, 124.90, 122.91, 122.36, 122.27, 120.82, 119.76, 115.30, 111.28, 109.02, 108.69, 105.95, 52.95, 43.97, 35.15, 13.39. **HRMS** (ESI) calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 499.1628, found 499.1626.

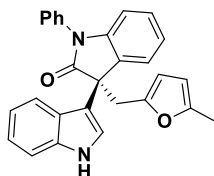


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	13.053	1164653	24980	50.956
2	17.813	1120968	12616	49.044
Total		2285621	37596	100.00



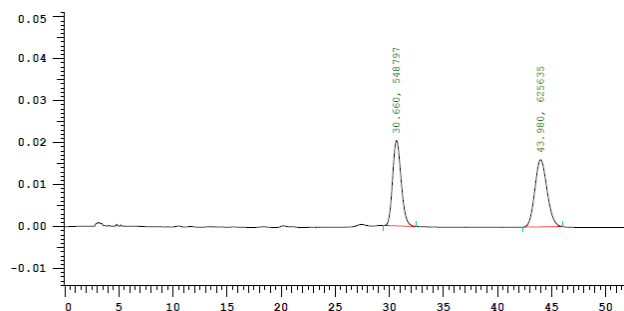
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	13.053	370209	7930	4.589
2	17.740	7696464	85607	95.411
Total		2285621	93537	100.00

(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-1-phenylindolin-2-one(3I)



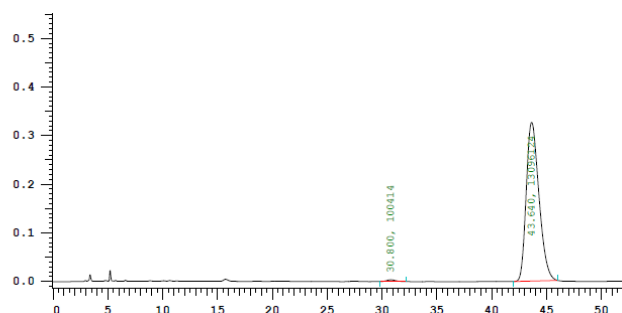
The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 78%; white solid; $[\alpha]_D^{20} = +17.6$ ($c = 0.31$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 80/20, flow rate 1.0 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 30.793$ min (minor), $t_R = 43.640$ min (major).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.26 (s, 1H), 7.48 (dd, $J = 13.8, 6.1$ Hz, 2H), 7.36 (t, $J = 7.4$ Hz, 1H), 7.32 – 7.27 (m, 4H), 7.25 – 7.22 (m, 2H), 7.19 (t, $J = 7.8$ Hz, 1H), 7.11 (t, $J = 7.7$ Hz, 1H), 7.05 (t, $J = 7.5$ Hz, 1H), 6.96 (dd, $J = 13.6, 5.7$ Hz, 1H), 6.76 (d, $J = 7.9$ Hz, 1H), 5.70 (d, $J = 2.1$ Hz, 1H), 5.66 (d, $J = 2.9$ Hz, 1H), 3.97 (d, $J = 14.2$ Hz, 1H), 3.62 (d, $J = 14.2$ Hz, 1H), 2.06 (s, 3H). **$^{13}\text{C NMR}$** (125 MHz, CDCl_3) δ 177.48, 150.84, 148.78, 143.83, 136.91, 134.82, 132.04, 129.45, 127.99, 127.87, 126.65, 125.59, 125.00, 122.96, 122.84, 122.23, 120.41, 119.81, 115.01, 111.38, 109.04, 108.52, 105.89, 53.12, 35.85, 13.40. **HRMS** (ESI) calcd for $\text{C}_{28}\text{H}_{22}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 441.1573, found 441.1576.



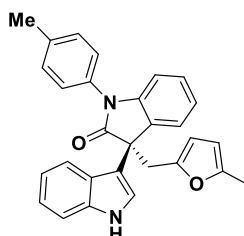
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	30.660	548797	10163	46.729
2	43.980	625635	7995	53.271

Total	1174432	18158	100.00
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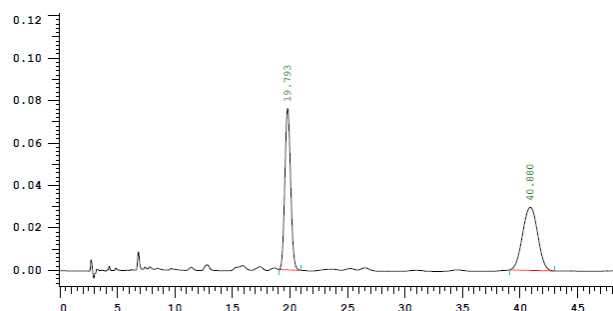
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	30.800	100414	1885	0.761
2	43.640	13096124	163109	99.239
Total		13196538	164994	100.00

(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-1-(p-tolyl)indolin-2-one(3m)



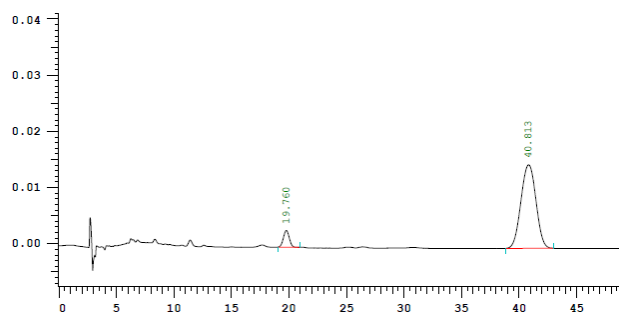
The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 64%; white solid; $[\alpha]_D^{20} = +19.3$ ($c = 0.29$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak IF, hexane/isopropanol/trifluoroacetic acid = 75/25/0.1, flow rate 1.0 mL/min, $T = 30^\circ\text{C}$, 250 nm, $t_R = 19.760$ min (minor), $t_R = 40.813$ min (major).

$^1\text{H NMR}$ (500 MHz, CDCl_3) δ 8.61 (s, 1H), 7.34 (d, $J = 8.2$ Hz, 1H), 7.28 (d, $J = 8.1$ Hz, 2H), 7.18 (dd, $J = 14.5, 7.5$ Hz, 5H), 7.11 (t, $J = 7.6$ Hz, 1H), 7.06 (d, $J = 2.6$ Hz, 1H), 7.05 – 7.01 (m, 1H), 6.96 – 6.91 (m, 1H), 6.73 (d, $J = 7.8$ Hz, 1H), 5.72 – 5.70 (m, 1H), 5.66 (d, $J = 3.0$ Hz, 1H), 3.92 (d, $J = 14.1$ Hz, 1H), 3.57 (d, $J = 14.1$ Hz, 1H), 2.40 (s, 3H), 2.07 (s, 3H). **$^{13}\text{C NMR}$** (125 MHz, CDCl_3) δ 177.96, 150.85, 148.79, 144.04, 137.92, 136.86, 132.19, 132.11, 130.15, 127.96, 126.53, 125.61, 124.91, 123.20, 122.84, 122.09, 120.10, 119.67, 114.59, 111.49, 109.02, 108.50, 105.90, 53.09, 35.77, 21.25, 13.43. **HRMS** (ESI) calcd for $\text{C}_{29}\text{H}_{24}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 455.1730, found 455.1731.



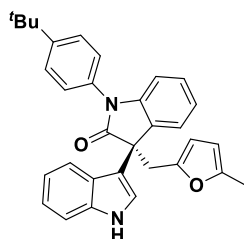
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	19.793	1312422	37956	49.374
2	40.880	1345725	14810	50.626

Total	2658147	52766	100.00
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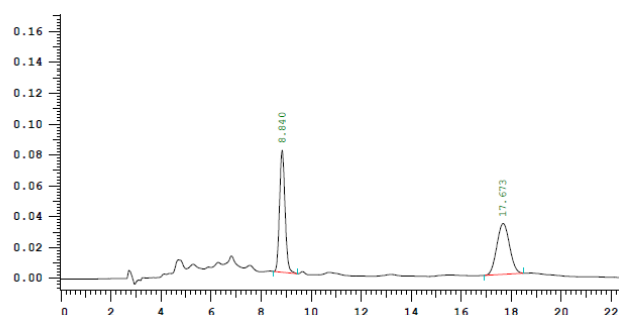
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	19.760	51577	1489	7.156
2	40.813	669165	7421	92.844
Total		720742	8910	100.00

(R)-1-(4-(tert-butyl)phenyl)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3n)



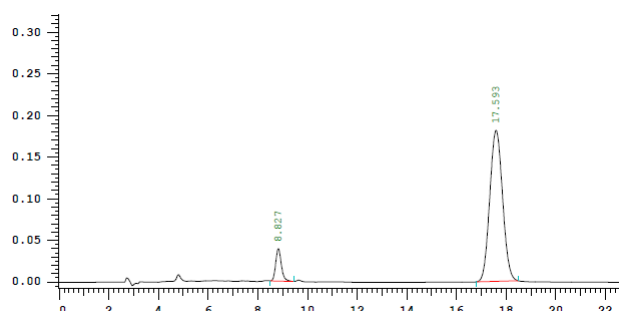
The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 51%; white solid; $[\alpha]_D^{20} = +26.8$ ($c = 0.20$, CHCl_3); The enantiomeric excess was determined by HPLC with Daicel Chirapak IF, hexane/isopropanol/trifluoroacetic acid = 75/25/0.1, flow rate 1.0 mL/min, $T = 30^\circ\text{C}$, 250 nm, $t_R = 8.827$ min (minor), $t_R = 17.593$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.57 (s, 1H), 7.51 – 7.47 (m, 2H), 7.35 (d, $J = 8.2$ Hz, 1H), 7.24 – 7.15 (m, 5H), 7.14 – 7.09 (m, 1H), 7.07 (d, $J = 2.6$ Hz, 1H), 7.03 (td, $J = 7.6, 0.7$ Hz, 1H), 6.96 – 6.91 (m, 1H), 6.78 (d, $J = 7.8$ Hz, 1H), 5.72 – 5.70 (m, 1H), 5.67 (d, $J = 3.0$ Hz, 1H), 3.93 (d, $J = 14.1$ Hz, 1H), 3.58 (d, $J = 14.2$ Hz, 1H), 2.08 (s, 3H), 1.35 (s, 9H). **^{13}C NMR** (125 MHz, CDCl_3) δ 177.95, 150.89, 150.83, 148.78, 143.98, 136.85, 132.19, 132.02, 127.92, 126.45, 126.10, 125.60, 124.89, 123.14, 122.84, 122.11, 120.15, 119.68, 114.69, 111.46, 109.14, 108.48, 105.89, 53.09, 35.74, 34.74, 31.37, 13.45. **HRMS** (ESI) calcd for $\text{C}_{32}\text{H}_{30}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 497.2199, found 497.2201.



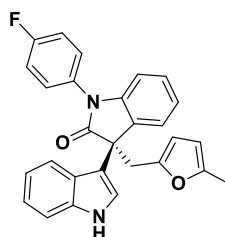
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
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1	8.840	609044	39469	51.150
2	17.673	581651	16463	48.850
Total		1190695	55932	100.00



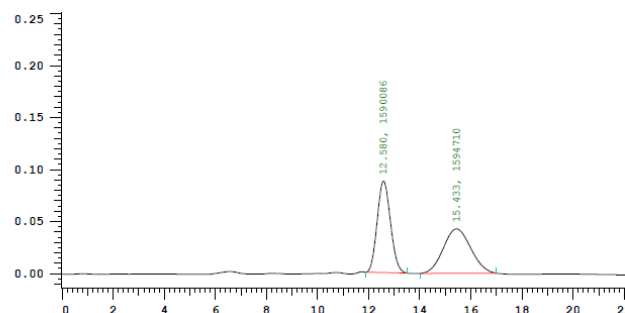
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	8.827	309024	19415	8.705
2	17.593	3241054	90534	91.295
Total		3550078	109949	100.00

(R)-1-(4-fluorophenyl)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3o)



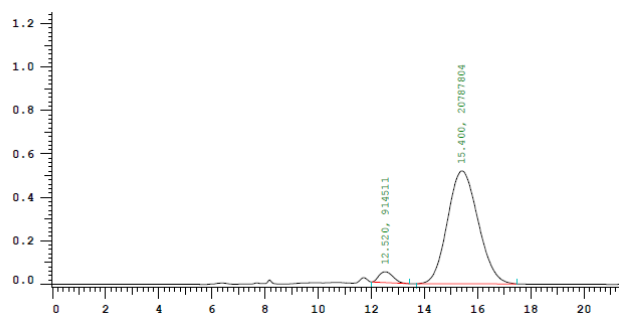
The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 92%; white solid; $[\alpha]_D^{20} = +36.9$ ($c = 0.27$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 70/30, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 12.527$ min (minor), $t_R = 15.400$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.37 (s, 1H), 7.34 (t, $J = 7.9$ Hz, 1H), 7.25 – 7.11 (m, 8H), 7.06 (dd, $J = 13.1, 5.6$ Hz, 1H), 6.95 (dd, $J = 14.7, 7.5$ Hz, 1H), 6.70 (d, $J = 7.8$ Hz, 1H), 5.71 (d, $J = 2.0$ Hz, 1H), 5.65 (d, $J = 3.0$ Hz, 1H), 3.99 – 3.93 (m, 1H), 3.59 (d, $J = 14.2$ Hz, 1H), 2.05 (d, $J = 7.0$ Hz, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 177.68, 150.88, 148.72, 143.73, 136.88, 131.98, 130.72, 130.69, 128.58, 128.51, 128.09, 125.56, 125.07, 123.03, 122.28, 120.25, 119.84, 116.56, 116.38, 114.73, 111.44, 108.82, 108.52, 105.90, 53.11, 35.84, 13.40. **HRMS** (ESI) calcd for $\text{C}_{28}\text{H}_{21}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 459.1479, found 459.1483;



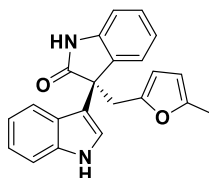
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	12.580	1590086	43923	49.927

2	15.433	1594710	21338	50.073
Total		3184796	65261	100.00



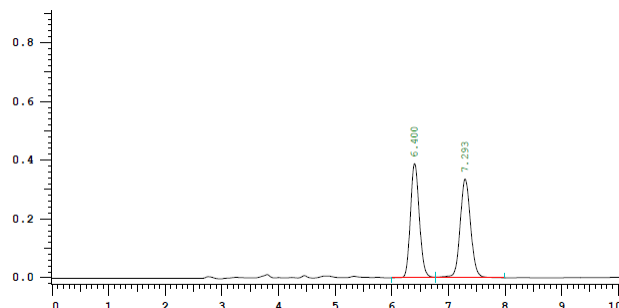
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	12.520	914511	24996	4.214
2	15.400	20787804	259621	95.786
Total		21702315	284617	100.00

(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3p)

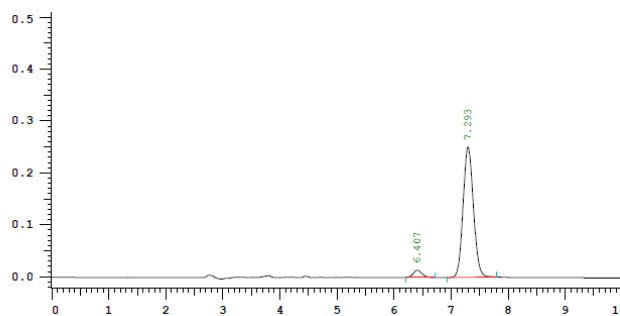


The product was isolated by flash column chromatography with petroleum ether/ethyl acetate = 10/1; yield: 51%; white solid; $[\alpha]_D^{20} = +51.8$ ($c = 0.29$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak IF, hexane/isopropanol/trifluoroacetic acid = 75/25/0.1, flow rate 1.0 mL/min, $T = 30^\circ\text{C}$, 250 nm, $t_R = 6.407$ min (minor), $t_R = 7.293$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 8.36 (s, 1H), 8.23 (s, 1H), 7.31 (d, $J = 8.1$ Hz, 1H), 7.18 (dd, $J = 15.8, 8.0$ Hz, 2H), 7.10 (d, $J = 8.2$ Hz, 3H), 6.98 (t, $J = 7.5$ Hz, 1H), 6.92 (t, $J = 7.5$ Hz, 1H), 6.83 (d, $J = 7.7$ Hz, 1H), 5.64 (s, 1H), 5.62 (d, $J = 2.4$ Hz, 1H), 3.80 (d, $J = 14.4$ Hz, 1H), 3.60 (d, $J = 14.4$ Hz, 1H), 2.03 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 180.41, 150.74, 148.65, 140.82, 136.84, 132.70, 128.15, 125.48, 125.24, 123.14, 122.40, 122.21, 120.36, 119.74, 114.55, 111.37, 109.57, 108.39, 105.92, 53.26, 35.07, 13.34. **HRMS** (ESI) calcd for $\text{C}_{22}\text{H}_{18}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 365.1260, found 365.1260.

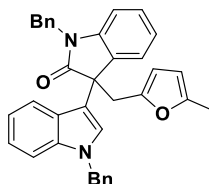


No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	6.400	2127180	194142	49.350
2	7.293	2183186	167838	50.650
Total		4310366	361980	100.00



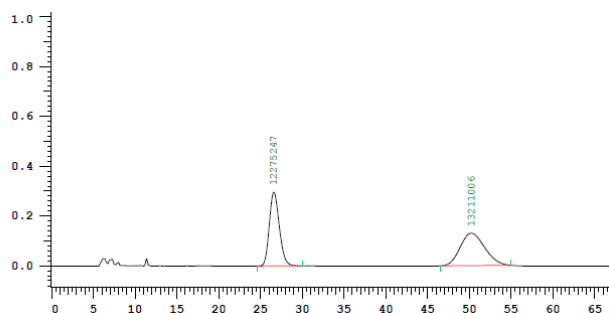
No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	6.407	75570	6974	4.556
2	7.293	1583278	125457	95.444
Total		1658848	132431	100.00

1-benzyl-3-(1-benzyl-5-chloro-1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(4)



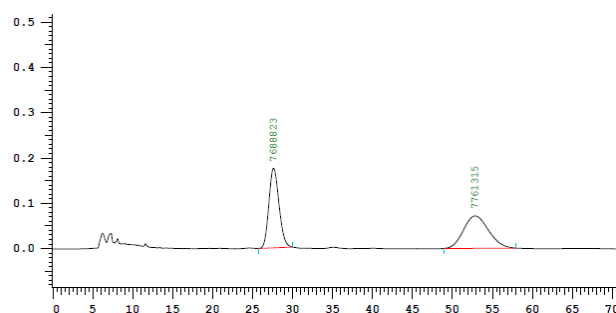
The product was isolated by flash column chromatography with petroleum ether = 10/1; yield: 35%; yellow oil; $[\alpha]_D^{20} = 0$ ($c = 0.35$, CHCl_3). The enantiomeric excess was determined by HPLC with Daicel Chirapak AS-H, hexane/isopropanol = 90/10, flow rate 0.5 mL/min, $T = 25^\circ\text{C}$, 250 nm, $t_R = 27.627$ min (minor), $t_R = 52.840$ min (major).

^1H NMR (500 MHz, CDCl_3) δ 7.30 (ddd, $J = 13.9, 11.4, 4.5$ Hz, 5H), 7.23 – 7.18 (m, 5H), 7.17 – 7.05 (m, 8H), 6.99 (dd, $J = 13.1, 5.7$ Hz, 1H), 6.92 (t, $J = 7.5$ Hz, 1H), 6.65 (d, $J = 7.8$ Hz, 1H), 5.67 (s, 1H), 5.56 (d, $J = 2.7$ Hz, 1H), 5.28 (s, 2H), 4.96 – 4.90 (m, 1H), 4.80 (d, $J = 15.8$ Hz, 1H), 3.89 (d, $J = 14.4$ Hz, 1H), 3.65 (d, $J = 14.4$ Hz, 1H), 2.03 (s, 3H). **^{13}C NMR** (125 MHz, CDCl_3) δ 178.04, 150.67, 148.83, 143.09, 137.35, 137.32, 135.86, 132.12, 128.80, 128.59, 128.09, 127.63, 127.35, 127.26, 127.14, 126.75, 126.29, 124.98, 122.34, 122.02, 121.10, 119.54, 114.21, 109.91, 109.04, 108.72, 105.94, 52.97, 50.15, 43.98, 35.25. **HRMS** (ESI) calcd for $\text{C}_{36}\text{H}_{30}\text{N}_2\text{NaO}_2$ $[\text{M}+\text{Na}]^+$ 545.2199, found: 545.2203.



No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	26.600	12275247	147944	48.164
2	50.240	13211006	65019	51.836

Total	25486253	212963	100.00
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No	Retention Time/min	Area/AU*100000*min	Height/AU*100000	Relative Area/%
1	27.627	7688823	87803	49.765
2	52.847	7761315	35770	50.235
Total		15450138	123573	100.00

5. DFT Calculations

5.1 Complete Reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

5.2 Computational Methods

All the DFT calculations were carried out with the GAUSSIAN 09 series of programs. DFT method B3-LYP² with a standard 6–31G(d) basis set was used for geometry optimizations. Harmonic vibrational frequency calculations were performed for all of the stationary points to confirm them as a local minima or transition structures, and to derive the thermochemical corrections for the enthalpies and free energies. The M11 functional in combination with the 6–311+G(d,p) basis set was used to calculate the solvation single point energies to give more accurate energy information. The solvent effects were considered by single point calculations on the gas-phase stationary points with an SMD³ solvation model in the DCE solvent.

² a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

³ Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

5.3 Free Energy Profiles for Alkylation C(sp³)-H Bond Functionalization of 2,5-Dimethylfuran with Indolyl Alcohols in the Absence of Phosphoric Acid

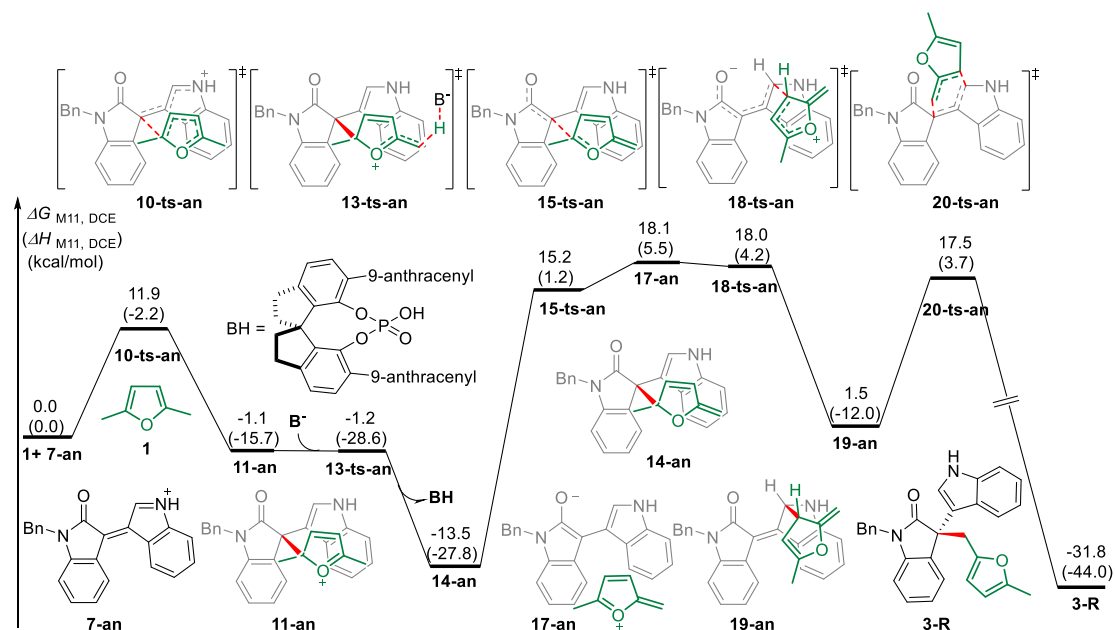


Fig S1. Free energy profiles for alkylation C(sp³)-H bond functionalization of 2,5-dimethylfuran with indolyl alcohols in the absence of phosphoric acid. The values given by kcal/mol are the relative free energies calculated by M11 method in DCE solvent.

5.4 Absolute Calculation Energies, Enthalpies, and Free Energies

Geometry	$E_{\text{(elec-B3LYP)}}^a$	$G_{\text{(corr-B3LYP)}}^b$	$H_{\text{(corr-B3LYP)}}^c$	$E_{\text{(solv, M11)}}^d$	IF ^e
1	-308.661143	0.095196	0.133939	-308.575786	-
BH	-2375.794985	0.569613	0.676817	-2375.228912	-
B⁻	-2375.270566	0.557451	0.663470	-2374.772569	-
5-ts	-2684.423878	0.681918	0.806743	-2683.776179	-639.30
6	-308.632088	0.095002	0.133113	-308.547107	-
7	-3447.025647	0.888895	1.043468	-3446.172442	-
8-ts	-3755.651487	1.003163	1.179004	-3754.730405	-289.36
9	-3755.674573	1.009742	1.180570	-3754.770179	-
10-ts	-3755.677430	1.009039	1.179896	-3754.759470	-274.77
11	-3755.686374	1.010939	1.181124	-3754.776338	-
13-ts	-6131.065985	1.59016	1.842144	-6129.570923	-834.10
14	-3755.267396	0.996059	1.167652	-3754.333024	-
15-ts	-3755.243007	0.994759	1.16525	-3754.300457	-170.95

16	-307.78253	0.085283	0.121301	-307.756279	-
17	-3447.319623	0.884476	1.041333	-3446.515168	-
18-ts	-3755.245401	0.994351	1.164906	-3754.297918	-201.38
19	-3755.263284	0.995011	1.167303	-3754.320739	-
20-ts	-3755.242927	0.995846	1.165258	-3754.293338	-310.34
3-R	-1379.48082	0.400906	0.489781	-1379.111904	-
21-ts	-3755.247843	0.993895	1.164816	-3754.292918	-209.55
22	-3755.262629	0.995472	1.167722	-3754.316369	-
23-ts	-3755.240789	0.995028	1.165433	-3754.290343	-305.80
3-S	-1379.48082	0.400906	0.489779	-1379.111904	-
24-ts	-3755.66371	1.007843	1.179245	-3754.739309	-295.03
25	-3755.676089	1.011239	1.180622	-3754.755258	-
26-ts	-6131.056529	1.589796	1.841096	-6129.543651	-1129.40
7-an	-1071.194535	0.294747	0.365472	-1070.918629	-
10-ts-an	-1379.843006	0.413122	0.499994	-1379.498574	-284.97
11-an	-1379.850908	0.415059	0.501333	-1379.521284	-
13-ts-an	-3755.239681	0.992085	1.163757	-3754.313509	-175.39
14-an	-1379.450321	0.402716	0.488192	-1379.084563	-
15-ts-an	-1379.418568	0.400145	0.486002	-1379.036149	-137.27
17-an	-1379.420315	0.398465	0.486671	-1379.02984	-
18-ts-an	-1379.420161	0.399631	0.485814	-1379.031172	-120.31
19-an	-1379.443017	0.401542	0.488414	-1379.059479	-
20-ts-an	-1379.421947	0.39988	0.486184	-1379.032247	-321.53

^aThe electronic energy calculated by B3LYP in gas phase. ^bThe thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ^cThe thermal correction to enthalpy calculated by B3LYP in gas phase. ^dThe electronic energy calculated by M11 in 1,2-dichloroethane solvent. ^eThe B3LYP calculated imaginary frequencies for the transition states.

5.5 B3LYP Geometries for All the Optimized Compounds and Transition State

1				H	1.40358200	5.40050400	-1.42480100
C	1.10847400	-0.00411400	0.00000500	H	0.91246300	4.66358800	-2.94638300
C	0.71796100	1.30156600	-0.00025200	O	-1.09544200	0.40488100	-0.62411800
C	-0.71797100	1.30155800	-0.00013700	O	1.15464700	0.40546400	0.64832300
C	-1.10846700	-0.00412700	0.00004700	P	-0.01557900	-0.58263000	0.07956400
O	0.00000500	-0.81300300	-0.00007900	O	-0.46947100	-1.48579100	1.14926500
H	1.37215500	2.16291500	-0.00042200	O	0.53327900	-1.21398300	-1.29102600
H	-1.37217300	2.16290100	-0.00020500	H	1.20263600	-1.90472300	-1.14436100
C	-2.43253500	-0.68492000	0.00018000	C	4.20397500	0.58426600	1.95253600
H	-2.56082500	-1.32308100	-0.88362600	C	4.28713800	-0.48103800	0.99908400
H	-2.56067300	-1.32303700	0.88403900	C	4.73591400	0.45977300	3.20943500
H	-3.23337400	0.06009500	0.00023000	C	3.74924800	-0.38307800	-0.30860500
C	2.43253500	-0.68491800	0.00015900	C	4.97012400	-1.68885700	1.40383800
H	3.23338800	0.06008300	-0.00007500	C	5.39296300	-0.73925400	3.60792900
H	2.56077600	-1.32281000	0.88416900	H	4.65752200	1.28452400	3.91259900
H	2.56070400	-1.32330600	-0.88349600	C	3.89518000	-1.46029500	-1.21894800
BH				C	5.10313700	-2.74196800	0.49444900
C	-1.82158400	3.29591000	1.53818600	C	5.50685200	-1.77998100	2.72645700
C	-1.20560600	2.49221000	0.56624800	H	5.80446400	-0.82020800	4.61022500
C	-1.78761400	1.27162900	0.23109700	C	3.36743900	-1.43039900	-2.55388700
C	-3.04334900	0.88908600	0.73770500	C	4.59001700	-2.65999800	-0.80269700
C	-3.66065800	1.75273700	1.65804800	H	5.62080900	-3.64769700	0.80355900
C	-3.04798300	2.93169800	2.08546800	H	6.01120200	-2.69926100	3.01435300
C	-0.95801300	4.49788500	1.85561100	C	3.52275000	-2.49387300	-3.40672800
C	0.39608200	4.11400000	1.21863400	H	2.82709200	-0.55036900	-2.88275500
C	0.01761000	3.20635800	-0.00054200	C	4.73446100	-3.74165200	-1.72785700
H	-4.62965700	1.46975700	2.05843300	C	4.21984500	-3.66553400	-2.99413800
H	-3.52920300	3.55512900	2.83483700	H	3.10799700	-2.44351500	-4.40976400
H	-1.36724800	5.41359800	1.40595800	H	5.26301300	-4.63235900	-1.39661200
H	0.98334000	3.52118400	1.92931700	H	4.33460400	-4.49565900	-3.68550100
H	0.99985900	4.97820900	0.92418100	C	-4.11550300	0.58114600	-1.97789900
H	-0.87927600	4.68515600	2.93256500	C	-4.25910300	-0.46031500	-1.00500200
C	-0.36136200	4.10464300	-1.22656500	C	-4.63091600	0.45620000	-3.24192500
H	-0.96424100	4.97129700	-0.93810300	C	-3.73983300	-0.36476800	0.31020600
H	-0.95006400	3.50685600	-1.93180200	C	-4.99236800	-1.64239200	-1.39755800
C	0.99176800	4.48301700	-1.86834000	C	-5.33452600	-0.71987500	-3.62875700
C	1.85469500	3.28232000	-1.54442500	H	-4.50464800	1.26355700	-3.95853200
C	1.24020000	2.48779400	-0.56295700	C	-3.94304300	-1.41622500	1.23654100
C	3.07844300	2.91441900	-2.09527400	C	-5.19655100	-2.66501700	-0.46686500
H	3.55672100	3.53376300	-2.84980400	C	-5.51056700	-1.73503200	-2.72753500
C	3.69111400	1.73562800	-1.66589100	H	-5.73359900	-0.80277100	-4.63611300
H	4.65805400	1.44870200	-2.06914100	C	-3.41901200	-1.39071400	2.56961600
C	3.07305800	0.88253200	-0.73797100	C	-4.69909600	-2.58190400	0.83620900
C	1.82046300	1.26863700	-0.22205300	H	-5.75993400	-3.54742400	-0.76419100

H	-6.05359000	-2.63558000	-3.00506800	O	0.61159300	-1.38480900	-1.19161700
C	-3.65433500	-2.41661500	3.44675400	C	4.18300600	0.62579500	1.93670300
H	-2.80538000	-0.55191200	2.87463200	C	4.35946600	-0.42722800	0.98241600
C	-4.92240400	-3.63005500	1.78368000	C	4.76753000	0.57709200	3.17579700
C	-4.42301900	-3.55002700	3.05530300	C	3.76922400	-0.39856500	-0.30639000
H	-3.23703400	-2.37450700	4.44914400	C	5.19777600	-1.54121000	1.36514600
H	-5.49884200	-4.49578800	1.46578000	C	5.57979500	-0.53045100	3.55244200
H	-4.59886800	-4.35303200	3.76617100	H	4.60661400	1.38836800	3.88155300
H	3.71283500	1.50690500	1.66528700	C	3.98858800	-1.47179700	-1.20330200
H	-3.59123300	1.48881800	-1.70082200	C	5.43707100	-2.56917300	0.44878200
B-				C	5.78771200	-1.55507700	2.66843100
C	-1.80325900	3.20770800	1.58330100	H	6.03210900	-0.55688700	4.54120000
C	-1.21031900	2.42673300	0.58269400	C	3.36352800	-1.53233100	-2.49090800
C	-1.77409600	1.19830100	0.21624400	C	4.85890900	-2.56180400	-0.82330500
C	-3.02623900	0.82169800	0.75499500	H	6.08716300	-3.39506300	0.73374100
C	-3.62295600	1.65259000	1.71816300	H	6.40872500	-2.40628800	2.94097300
C	-3.01092000	2.82605100	2.16127700	C	3.62969000	-2.55761700	-3.36000700
C	-0.94131900	4.41372000	1.89495800	H	2.62973000	-0.77799000	-2.74130900
C	0.39833200	4.04824000	1.21742800	C	5.11166000	-3.61126100	-1.76257500
C	0.00003600	3.14772600	0.00019900	C	4.52596600	-3.60491300	-2.99980400
H	-4.57996400	1.35190300	2.13723300	H	3.12833800	-2.59061300	-4.32381900
H	-3.47497500	3.42768100	2.94006100	H	5.77751700	-4.41895600	-1.46467000
H	-1.36739300	5.33356600	1.46620800	H	4.72354300	-4.41062700	-3.70354500
H	1.00570700	3.44897600	1.90530700	C	-4.18339900	0.62618700	-1.93640200
H	0.99001600	4.92129600	0.91931600	C	-4.35965100	-0.42703300	-0.98231500
H	-0.83606100	4.59058500	2.97276400	C	-4.76823500	0.57780200	-3.17534100
C	-0.39818900	4.04851600	-1.21682600	C	-3.76916300	-0.39866800	0.30637200
H	-0.98985000	4.92152700	-0.91853700	C	-5.19808300	-1.54090500	-1.36510200
H	-1.00556300	3.44944400	-1.90487100	C	-5.58064300	-0.52961200	-3.55204800
C	0.94149900	4.41410800	-1.89424600	H	-4.60747700	1.38923300	-3.88095100
C	1.80343800	3.20804400	-1.58275600	C	-3.98838800	-1.47206400	1.20312400
C	1.21041100	2.42683100	-0.58239200	C	-5.43718500	-2.56908600	-0.44893400
C	3.01118300	2.82657600	-2.16067900	C	-5.78836000	-1.55444900	-2.66824000
H	3.47530500	3.42840900	-2.93926200	H	-6.03323800	-0.55577700	-4.54068400
C	3.62321600	1.65303800	-1.71776600	C	-3.36315600	-1.53284500	2.49063400
H	4.58030500	1.35248000	-2.13675100	C	-4.85876700	-2.56200300	0.82304600
C	3.02639800	0.82189400	-0.75488800	H	-6.08732900	-3.39492400	-0.73394600
C	1.77414900	1.19830400	-0.21620100	H	-6.40947800	-2.40557600	-2.94082300
H	1.36755600	5.33390300	-1.46538300	C	-3.62917200	-2.55830900	3.35957500
H	0.83626000	4.59109700	-2.97203400	H	-2.62938600	-0.77850200	2.74111100
O	-1.11484400	0.39129200	-0.66051300	C	-5.11134000	-3.61168100	1.76212900
O	1.11481500	0.39095900	0.66016500	C	-4.52545500	-3.60557300	2.99928100
P	-0.00004400	-0.73324600	-0.00047800	H	-3.12772800	-2.59146800	4.32333900
O	-0.61170800	-1.38535000	1.19038000	H	-5.77721300	-4.41934200	1.46416100

H	-4.72288100	-4.41146100	3.70287200	C	5.52933200	0.16335400	3.70638200
H	3.56566100	1.47344000	1.66409100	H	4.90299900	2.24322000	3.58951900
H	-3.56595100	1.47373500	-1.66375900	C	3.87840100	-1.46689500	-0.84016800
5-ts				C	5.07619100	-2.42371400	1.08001200
C	-1.35839100	4.30301800	0.80195700	C	5.57121000	-1.04246900	3.06021300
C	-0.83403500	3.24674200	0.04172600	H	5.96005100	0.27070600	4.69837600
C	-1.51926300	2.03344500	-0.01040900	C	3.29777000	-1.68958600	-2.13142300
C	-2.79690600	1.90043700	0.57132000	C	4.53444500	-2.58490800	-0.19846600
C	-3.32486600	3.00236800	1.26379700	H	5.56765300	-3.26823800	1.55973500
C	-2.60440500	4.18908200	1.41149200	H	6.03772600	-1.90691600	3.52737600
C	-0.38290600	5.46050200	0.84143600	C	3.39780800	-2.90464400	-2.75867800
C	0.91943400	4.81838000	0.31223900	H	2.74894700	-0.88236000	-2.59975700
C	0.43805100	3.69713600	-0.66954300	C	4.61587800	-3.83693000	-0.88743300
H	-4.30907300	2.90779800	1.71408200	C	4.07422200	-3.99368000	-2.13552000
H	-3.01660000	5.00899000	1.99452600	H	2.94951500	-3.04306700	-3.73921000
H	-0.71441900	6.28489000	0.19400500	H	5.12678900	-4.66187700	-0.39558600
H	1.46324400	4.35034200	1.14084200	H	4.15343900	-4.94697300	-2.65241100
H	1.59360600	5.53483000	-0.16827100	C	-3.88698900	0.99933500	-2.00294900
H	-0.26857400	5.87896000	1.84814900	C	-4.10990400	0.24570000	-0.80547900
C	0.11520900	4.32785700	-2.06669100	C	-4.39097300	0.59190400	-3.21062400
H	-0.39921900	5.29051900	-1.98228700	C	-3.59373800	0.63898900	0.45488000
H	-0.54153200	3.64375300	-2.61642900	C	-4.91332400	-0.95149900	-0.91008000
C	1.48165200	4.42039100	-2.78038800	C	-5.16309700	-0.60083700	-3.31135900
C	2.23275600	3.24247100	-2.19761900	H	-4.20337900	1.18424200	-4.10216000
C	1.57567100	2.75641100	-1.05696000	C	-3.87669900	-0.13517400	1.60741000
C	3.39599400	2.63598900	-2.66173900	C	-5.19218100	-1.69588100	0.23936400
H	3.90912900	3.01548700	-3.54194600	C	-5.41873000	-1.34478900	-2.19012400
C	3.89970000	1.52752300	-1.97950300	H	-5.55667500	-0.90818800	-4.27676400
H	4.81887200	1.05630800	-2.31626600	C	-3.35706200	0.18722400	2.90380200
C	3.23238100	0.97557000	-0.87353200	C	-4.70170000	-1.31745800	1.49190300
C	2.04042500	1.59330200	-0.44209200	H	-5.80856800	-2.58932400	0.15775200
H	1.98841700	5.36910000	-2.55237100	H	-6.02369600	-2.24717200	-2.24866500
H	1.39413000	4.36546200	-3.87170200	C	-3.65747900	-0.57485300	4.00282900
O	-0.93535300	0.94860200	-0.64216700	H	-2.69153200	1.03557800	3.00000300
O	1.31874800	1.04499800	0.60564200	C	-4.99184000	-2.08547500	2.66448400
P	0.09799300	-0.00653400	0.23080500	C	-4.49238600	-1.72403700	3.88748300
O	-0.51616400	-0.31790000	1.59781600	H	-3.24418600	-0.30941800	4.97213900
O	0.51889300	-1.11950300	-0.66779300	H	-5.62347400	-2.96488400	2.55972200
H	1.15297000	-3.15611800	-0.10346400	H	-4.72380000	-2.31319100	4.77118900
C	4.37267600	1.17462700	1.82431300	H	3.92144900	2.04131600	1.35559900
C	4.37828200	-0.06888300	1.11365500	H	-3.30684100	1.91271900	-1.94282900
C	4.92464200	1.28699200	3.07364500	C	-1.38735000	-4.12490800	-1.39725700
C	3.81665500	-0.21541400	-0.17934400	C	-0.08627200	-4.40408400	-1.35636700
C	5.00961500	-1.20102100	1.75394400	C	0.45427700	-4.00173700	-0.01600300

C	-0.78039000	-3.50808900	0.67314100	C	5.66832100	-0.15335000	-2.65670700
O	-1.81456000	-3.59726300	-0.14027100	H	6.71792000	0.12367900	-2.52073000
H	0.50785900	-4.79302200	-2.17052600	H	5.10772700	0.76044300	-2.88476900
H	0.94654800	-4.80299100	0.55025900	C	5.44995900	-1.19482800	-3.77844700
C	-0.92592300	-2.91733000	1.93995800	C	4.17767800	-1.88841800	-3.34091400
H	-0.71995200	-1.67765300	1.73725400	C	3.87869100	-1.56389300	-2.00653700
H	-1.94007500	-2.92173600	2.34149100	C	3.33759900	-2.71838900	-4.07712000
H	-0.14777600	-3.18448800	2.65500500	H	3.57767900	-2.97949500	-5.10429800
C	-2.46665800	-4.21650000	-2.41089300	C	2.17555700	-3.21731300	-3.48339100
H	-2.06267800	-4.60590800	-3.34877100	H	1.52756300	-3.88747400	-4.04068300
H	-3.27079300	-4.88123000	-2.07217600	C	1.80223600	-2.84614100	-2.18220000
H	-2.90816300	-3.23064000	-2.59777000	C	2.66664400	-1.98871400	-1.47461600
6				H	6.28858800	-1.90175800	-3.83804400
H	1.28087300	1.80558800	0.88085300	H	5.35536800	-0.73570700	-4.76854800
C	1.17608100	-0.18686300	0.00007300	O	2.68111500	0.97904000	-0.56312800
C	0.85791800	1.30203700	0.00003900	O	2.26787400	-1.53706000	-0.20734700
C	-0.65094900	1.28110300	-0.00005800	P	1.56915300	-0.08110300	-0.07789700
C	-1.06503100	0.01107500	0.00018000	O	1.01963900	0.07015700	1.29398600
O	-0.01752300	-0.90135300	0.00028900	O	0.56471200	0.07932500	-1.29900900
H	1.28093100	1.80545600	-0.88086600	H	-0.39233000	0.11893600	-1.08508700
H	-1.28933600	2.15411200	-0.00009400	C	1.84033800	-4.74730800	0.04978800
C	-2.41966900	-0.60592100	-0.00016500	C	0.60230400	-4.25713200	-0.47326800
H	-2.55688000	-1.24188600	-0.88323300	C	1.87335600	-5.62405800	1.10487400
H	-2.55732900	-1.24213100	0.88261900	C	0.53606300	-3.35290900	-1.56639900
H	-3.19290400	0.16664800	-0.00031600	C	-0.61680500	-4.73515200	0.13714400
C	2.35028300	-0.81594200	-0.00018500	C	0.66971400	-6.07460100	1.71468500
H	3.27549000	-0.25127600	-0.00042500	H	2.82803200	-5.98649300	1.47537700
H	2.40754700	-1.89861500	-0.00015900	C	-0.72386800	-2.95450600	-2.08004100
7				C	-1.85121500	-4.31723500	-0.37253600
C	6.09847100	0.15876900	0.55033400	C	-0.54043200	-5.64102700	1.23977900
C	4.92348800	0.16552500	-0.21959000	H	0.71595000	-6.77189000	2.54641200
C	3.89838400	1.03756600	0.13685500	C	-0.86402800	-2.05421200	-3.18591900
C	4.04205600	1.97488900	1.17583600	C	-1.93665500	-3.45732100	-1.47122000
C	5.26017200	1.98217900	1.87577700	H	-2.76604000	-4.69008800	0.08348000
C	6.27572200	1.06961500	1.58736300	H	-1.46873200	-5.98933800	1.68602100
C	7.02395600	-0.94783300	0.09515200	C	-2.09960200	-1.71294800	-3.67966100
C	6.09120100	-1.82505400	-0.76673900	H	0.02856700	-1.63848800	-3.63745700
C	5.05508100	-0.81979300	-1.37916800	C	-3.20360300	-3.07023900	-2.00945600
H	5.39185900	2.70416900	2.67612600	C	-3.28688500	-2.23205200	-3.09258800
H	7.19075500	1.07053800	2.17363800	H	-2.17047300	-1.04470800	-4.53357500
H	7.85922200	-0.54976400	-0.49710500	H	-4.10274900	-3.48098500	-1.55614800
H	5.55750400	-2.53633800	-0.12557900	H	-4.25554700	-1.96967800	-3.50958300
H	6.61970100	-2.39903400	-1.53354100	C	3.26224700	4.20394000	-0.58470000
H	7.46646100	-1.49709700	0.93333400	C	2.62161900	4.00227200	0.67975400

C	2.91121400	5.24477300	-1.40572600	H	-6.12250400	3.51421300	-3.21162600
C	2.95729600	2.93596700	1.55062200	C	-3.94061900	5.90873100	-2.17786800
C	1.60609800	4.95254200	1.07405700	H	-1.92386000	5.53368400	-1.49938700
C	1.89771700	6.16733900	-1.01990700	H	-5.96520000	5.96436000	-2.91945900
H	3.41606800	5.37430400	-2.35896000	H	-3.86960100	6.98621200	-2.05929700
C	2.30473600	2.80452800	2.80193100	O	-2.16112000	0.55469900	-0.95401200
C	0.98325000	4.81759200	2.31847100	C	-2.86139900	-3.62871600	4.71679800
C	1.26904800	6.02434000	0.18883400	C	-4.09242700	-3.58741300	4.05023600
H	1.63929300	6.98998800	-1.68075900	C	-4.31738600	-2.70151100	2.99225900
C	2.57506100	1.73136400	3.71167800	C	-3.29385800	-1.82941000	2.60600600
C	1.30712900	3.77519200	3.19183400	C	-2.04845900	-1.92386200	3.27684200
H	0.23171300	5.54570900	2.61709000	C	-1.80651300	-2.79800800	4.32608900
H	0.50885900	6.73422900	0.50665600	H	-2.71686000	-4.32358900	5.53792300
C	1.93698200	1.64346200	4.92306600	H	-4.88872000	-4.25792900	4.35792000
H	3.29674000	0.97514900	3.42661700	H	-5.26729700	-2.72060300	2.47234900
C	0.66702400	3.64904800	4.46486400	H	-0.83850100	-2.84439300	4.81466800
C	0.97439700	2.61823500	5.31266000	C	-1.75442500	-0.40657300	1.65412800
H	2.17217100	0.82480900	5.59849600	C	-3.11778000	-0.83647200	1.53758500
H	-0.06891100	4.39831400	4.74689100	N	-1.16370400	-1.02303600	2.65817800
H	0.48861000	2.54005400	6.28146500	H	-0.17651500	-0.85407800	2.85225400
H	2.76768500	-4.42736100	-0.41080700	H	-1.22532500	0.34367400	1.09676000
H	4.04662200	3.52069400	-0.89039000	8-ts			
C	-7.95624200	0.46722000	-0.37861600	H	6.72733600	-1.61443700	-2.10956100
C	-7.74060900	-0.22376300	0.82361600	C	4.99125700	-1.58738300	-0.84061400
C	-6.44912300	-0.54203500	1.22697100	C	6.46805700	-1.44935900	-1.05229800
C	-5.36108100	-0.17973700	0.41017000	C	7.00393500	-2.51236300	-0.13758400
C	-5.60647500	0.55769300	-0.78690100	C	5.97953000	-3.14322200	0.44223100
C	-6.89325900	0.87765200	-1.19318600	O	4.74505400	-2.59054500	-0.00423600
H	-8.97123100	0.70929600	-0.67952600	H	6.80677800	-0.42902100	-0.81630200
H	-8.58558200	-0.50044000	1.44514700	H	8.05059300	-2.74005000	0.00813300
H	-6.28564700	-1.03868900	2.17494700	C	5.83994000	-4.25095500	1.41862500
H	-7.07923400	1.44523300	-2.09737400	H	5.28605900	-3.91712600	2.30343500
C	-3.34448100	0.42381300	-0.65119000	H	5.29426300	-5.09421000	0.97975000
C	-3.94177500	-0.28632400	0.56491900	H	6.82726100	-4.59975200	1.73008500
N	-4.39535100	0.88586200	-1.40205200	C	3.94261900	-0.76741000	-1.25957200
C	-4.20941300	1.62283600	-2.66517600	C	-5.50552900	-3.24055600	-0.28066400
H	-3.28819300	1.22832700	-3.10069100	C	-4.75793000	-2.12198400	-0.68394500
H	-5.03631300	1.34844000	-3.32624900	C	-3.39197500	-2.26860100	-0.91092900
C	-4.12298700	3.12725100	-2.49345900	C	-2.76634900	-3.52829800	-0.84585300
C	-2.93926000	3.71226100	-2.01981700	C	-3.56546900	-4.63705300	-0.51798800
C	-5.20709100	3.95079100	-2.81736100	C	-4.91918500	-4.50020500	-0.21091100
C	-2.84991600	5.09456600	-1.86046600	C	-6.92214400	-2.83557400	0.06240500
H	-2.08593700	3.08258800	-1.78401800	C	-6.80964400	-1.29932300	0.17034000
C	-5.11830700	5.33560600	-2.65979500	C	-5.67638400	-0.91445700	-0.84183000

H	-3.09884300	-5.61683600	-0.47772900	C	-0.28327700	5.90116200	-0.15872500
H	-5.50129700	-5.36877500	0.08535800	H	-0.99842500	5.35366100	-2.14136400
H	-7.62379300	-3.13221000	-0.72928800	H	0.23240300	6.20310600	1.89620300
H	-6.48979800	-1.02262900	1.18158500	H	0.41977900	6.64115400	-0.53309800
H	-7.74919000	-0.77872200	-0.03636700	C	-1.57239300	-3.11981500	-3.51031700
H	-7.27790200	-3.30089400	0.98823400	C	-0.77371900	-3.54582100	-2.40055800
C	-6.27633100	-0.83143100	-2.28590900	C	-1.03047400	-2.95240700	-4.75787500
H	-6.97676100	-1.64538700	-2.49544000	C	-1.30634900	-3.73175300	-1.10050200
H	-5.45897700	-0.89763200	-3.01337700	C	0.62454400	-3.82051300	-2.64838300
C	-6.92394900	0.56880100	-2.35418700	C	0.35166900	-3.20525800	-4.99131800
C	-6.04949200	1.37906600	-1.42205500	H	-1.66109600	-2.63145200	-5.58210200
C	-5.23339400	0.53453400	-0.65063100	C	-0.47208800	-4.19526600	-0.05184900
C	-5.97464000	2.76109800	-1.28437200	C	1.42685400	-4.29847800	-1.60691300
H	-6.61766700	3.41340800	-1.86933300	C	1.15148100	-3.63001100	-3.96486000
C	-5.06399600	3.30515500	-0.37860900	H	0.76114700	-3.07343600	-5.98902500
H	-5.01604400	4.38109900	-0.24070600	C	-0.93826200	-4.36805500	1.29371500
C	-4.17167100	2.49887800	0.34847000	C	0.91305800	-4.50792300	-0.32321200
C	-4.26054200	1.10542600	0.16706800	H	2.46916800	-4.54039900	-1.80743600
H	-7.96574100	0.54624900	-2.00613800	H	2.20344000	-3.84835000	-4.13520400
H	-6.94159100	0.97706700	-3.37077700	C	-0.12138000	-4.87049900	2.27638800
O	-2.62844400	-1.12890200	-1.19741100	H	-1.95853200	-4.09273600	1.53054500
O	-3.34484200	0.27671800	0.83615900	C	1.72837300	-5.03617800	0.72778400
P	-2.04352300	-0.29212000	0.07071700	C	1.22900800	-5.22771000	1.98788400
O	-1.17224700	-1.05835900	0.99172500	H	-0.51084000	-5.01206300	3.28135600
O	-1.41463400	0.96092500	-0.67999400	H	2.75819400	-5.29581800	0.49387200
H	-0.43290900	0.93272100	-0.74750000	H	1.85497100	-5.64617600	2.77139600
C	-4.32934000	2.10316400	3.26343200	H	-5.04474800	1.61410900	2.61265000
C	-3.31763700	2.93429900	2.68310300	H	-2.62891000	-2.93644700	-3.35442100
C	-4.41866000	1.92678000	4.61965600	C	6.36753300	3.56444900	0.26568400
C	-3.19609300	3.13890500	1.28500700	C	6.78871700	2.37192600	0.85753900
C	-2.41300800	3.61031300	3.58580500	C	5.92599300	1.27029500	0.91977600
C	-3.50485500	2.57152800	5.50118200	C	4.63562900	1.37652700	0.40002100
H	-5.19960400	1.29293200	5.03069400	C	4.24490400	2.58169100	-0.21741400
C	-2.20906300	4.02250600	0.77976800	C	5.08744200	3.68356200	-0.28908700
C	-1.45530900	4.48859500	3.07091900	H	7.04374000	4.41284300	0.22277000
C	-2.53421300	3.39245800	4.99436500	H	7.78952600	2.29555100	1.27060100
H	-3.59143300	2.41841200	6.57323500	H	6.26874100	0.34430900	1.36860800
C	-2.02231300	4.26525900	-0.62137800	H	4.77571500	4.60248000	-0.77117400
C	-1.34090200	4.72496900	1.69855800	C	2.43722800	1.21225900	-0.50421300
H	-0.79581900	5.01559700	3.75756900	C	3.50411500	0.41502700	0.28838800
H	-1.84041000	3.90615400	5.65552300	N	2.93566600	2.46264800	-0.72110100
C	-1.10206200	5.17660900	-1.07386700	C	2.19570100	3.50718100	-1.44541100
H	-2.62657200	3.71394300	-1.33174100	H	1.14386200	3.21607800	-1.39953900
C	-0.39079300	5.66468600	1.18580100	H	2.29449300	4.43901000	-0.88186700

C	2.65348600	3.68129900	-2.88117800	C	4.94141000	-0.83895700	-0.85520000
C	2.50489100	2.63243900	-3.80103200	C	3.80081200	-1.55876800	-0.51194200
C	3.20241300	4.89255300	-3.31489300	C	3.50139700	-2.79767400	-1.10896800
C	2.91238400	2.79218100	-5.12474800	C	4.37767500	-3.26867200	-2.10220100
H	2.04921300	1.69816200	-3.48132500	C	5.47290900	-2.51761700	-2.52973200
C	3.60652900	5.05569100	-4.64247300	C	6.83119500	-0.29747000	-2.22890800
H	3.30348100	5.72070100	-2.61628300	C	6.36058100	0.95871500	-1.46290200
C	3.46635800	4.00407800	-5.54815500	C	5.58063100	0.39464300	-0.22712700
H	2.78559200	1.97624500	-5.83100000	H	4.17125300	-4.23132900	-2.56016900
H	4.02764000	6.00318300	-4.96639200	H	6.10486700	-2.88546800	-3.33370100
H	3.77838800	4.12914900	-6.58105000	H	7.80855700	-0.64577700	-1.86804500
O	1.34966500	0.79667400	-0.89815900	H	5.66795600	1.53564100	-2.08672600
C	3.72891500	-1.75941300	5.32694200	H	7.17926000	1.62317900	-1.17184700
C	4.69860000	-0.89456200	4.79605400	H	6.93895100	-0.12175900	-3.30495100
C	4.58660400	-0.37476200	3.50689100	C	6.60220100	-0.00768100	0.89061600
C	3.48553900	-0.72875900	2.70852200	H	7.48629800	-0.50989400	0.48714500
C	2.50564000	-1.58024200	3.29235400	H	6.11190000	-0.69991100	1.58482800
C	2.60655600	-2.10550900	4.57826900	C	6.92276400	1.31657600	1.61534700
H	3.84337700	-2.14600600	6.33491100	C	5.63125900	2.08972700	1.46454400
H	5.55157800	-0.61229900	5.40620000	C	4.80453400	1.48990200	0.49910600
H	5.33561800	0.32169400	3.15694700	C	5.21689400	3.22507500	2.15242700
H	1.83112300	-2.74893000	4.98277300	H	5.86286900	3.69537900	2.88894800
C	1.74673200	-1.04871300	1.25633100	C	3.95530800	3.75641800	1.88682500
C	2.98720200	-0.38977700	1.37155100	H	3.62671600	4.65429100	2.40149600
N	1.47831800	-1.73573700	2.36883500	C	3.06840800	3.13980900	0.98831600
H	0.61990100	-2.26578100	2.48671400	C	3.51412200	1.98383000	0.32017700
H	1.03651500	-1.04718800	0.44902100	H	7.76100400	1.84295300	1.13851000
H	2.95857400	-1.21920700	-1.33313600	H	7.20108100	1.16807500	2.66440400
H	4.18523700	-0.06824600	-2.05615100	O	2.93070200	-1.04206000	0.45863300
9				O	2.62926200	1.31442300	-0.54424500
H	-2.37259200	-0.26575700	-3.40117600	P	1.80741200	0.02313900	-0.00678500
C	-2.62826100	-1.78522500	-1.96465400	O	0.84678600	-0.41119900	-1.05811600
C	-2.23621400	-1.36124500	-3.32144100	O	1.22096400	0.36064100	1.42547300
C	-3.11721500	-2.20725000	-4.18217700	H	0.27292600	0.64189100	1.39784500
C	-3.85457900	-2.99708600	-3.39667600	C	2.31154100	4.38484500	-1.57070000
O	-3.53197400	-2.71601400	-2.02260100	C	1.40632600	4.36713200	-0.45978300
H	-1.15455500	-1.53267100	-3.46795200	C	1.98333000	4.99450600	-2.75402700
H	-3.13581500	-2.19492300	-5.26285800	C	1.71552000	3.74287900	0.77470300
C	-4.87195100	-4.05907500	-3.58001800	C	0.13948200	5.04471300	-0.61956600
H	-4.51413300	-5.01539500	-3.18128900	C	0.72702500	5.65055400	-2.91087200
H	-5.80290500	-3.80679800	-3.06018000	H	2.69171100	4.99322300	-3.57773300
H	-5.08688100	-4.18363900	-4.64397100	C	0.78177300	3.77607600	1.84153400
C	-2.23788300	-1.21192500	-0.68291500	C	-0.76558400	5.07726000	0.44492800
C	5.74168100	-1.29945300	-1.91397900	C	-0.16143600	5.68046000	-1.86683100

H	0.49258900	6.14788600	-3.84835100	H	-5.46342700	-0.66174100	-1.93669400
C	1.02305000	3.14646600	3.10699800	H	-6.08133500	-0.48901200	3.01967400
C	-0.47966500	4.46205300	1.66664900	C	-2.55367900	0.47318300	1.08383500
H	-1.71301900	5.59708400	0.32033400	C	-3.09608400	0.12240500	-0.34199800
H	-1.11348800	6.19711300	-1.96185000	N	-3.54840800	0.25720400	1.98942100
C	0.10514700	3.21316000	4.12338200	C	-3.35230500	0.43263400	3.43668500
H	1.94776900	2.60170800	3.25395200	H	-2.52212000	1.13736300	3.53553000
C	-1.40890700	4.50925300	2.75313500	H	-4.24964100	0.91178600	3.83994900
C	-1.12562900	3.91059500	3.95170100	C	-3.05923800	-0.86863700	4.16048800
H	0.31840300	2.73108300	5.07355100	C	-1.87521500	-1.57310200	3.89335300
H	-2.34397300	5.04438100	2.60617600	C	-3.95479800	-1.37862300	5.10620700
H	-1.83117500	3.96942800	4.77621400	C	-1.60524200	-2.77373500	4.54889300
C	3.18687000	-3.96468800	1.58528400	H	-1.15572400	-1.17217100	3.18396700
C	2.19469000	-4.16167600	0.57189000	C	-3.68157700	-2.57703300	5.77043700
C	3.04820400	-4.50723200	2.83618400	H	-4.86700100	-0.83210800	5.33678500
C	2.30503500	-3.60932200	-0.72982700	C	-2.50945700	-3.27884000	5.48813000
C	1.05611400	-4.98831100	0.90447600	H	-0.68590800	-3.31051900	4.33043700
C	1.90842900	-5.29437500	3.16723000	H	-4.38397600	-2.95917500	6.50580500
H	3.81854600	-4.34275800	3.58414200	H	-2.29632400	-4.21126500	6.00336800
C	1.31498900	-3.89046800	-1.70464100	O	-1.41946900	0.84982800	1.35042500
C	0.10094900	-5.27299000	-0.07636700	C	-4.91410100	4.58053800	-2.95004100
C	0.94420500	-5.53022400	2.22368800	C	-5.69943500	3.70543600	-2.17361700
H	1.81984800	-5.72080000	4.16251400	C	-5.15463600	2.57586700	-1.57643600
C	1.35481100	-3.35079300	-3.03279000	C	-3.78287100	2.29456500	-1.74939000
C	0.21170800	-4.76446800	-1.37311500	C	-3.01208000	3.20883000	-2.52248200
H	-0.73352300	-5.92638900	0.17030700	C	-3.55868400	4.34292300	-3.13283600
H	0.08097500	-6.14965100	2.45459000	H	-5.37298900	5.45263600	-3.40633600
C	0.43251900	-3.71330300	-3.98306800	H	-6.75523100	3.92065800	-2.03625800
H	2.14174100	-2.65204300	-3.28923500	H	-5.78599300	1.93213200	-0.97716300
C	-0.73480200	-5.11126200	-2.39022600	H	-2.94060700	5.01211900	-3.72429700
C	-0.61837300	-4.62346800	-3.66570700	C	-1.60798800	1.61956700	-1.78039000
H	0.51490600	-3.31850800	-4.99274600	C	-2.85909700	1.26639800	-1.29397900
H	-1.53202500	-5.80481400	-2.13117600	N	-1.70736700	2.75633200	-2.53244100
H	-1.31622800	-4.93201800	-4.43914800	H	-0.91800700	3.28658800	-2.87857800
H	3.27976100	3.90948100	-1.46477800	H	-0.64981200	1.13555600	-1.63575300
H	4.06922000	-3.38145900	1.35021900	H	-1.17535800	-0.93556900	-0.70459900
C	-6.98582200	-0.92249300	1.10160800	H	-2.42336500	-1.93516000	0.11585600
C	-6.81496800	-0.97912500	-0.28316800	10-ts			
C	-5.58014700	-0.64696800	-0.85647600	C	6.07783200	0.28667500	1.65020100
C	-4.53168400	-0.25363800	-0.03243100	C	5.13038700	0.11570200	0.62702800
C	-4.72693000	-0.19175100	1.35699400	C	4.06965800	1.01425500	0.53717100
C	-5.94128900	-0.52561200	1.94542700	C	3.99071200	2.15176100	1.36362900
H	-7.94515400	-1.18599000	1.53686100	C	5.00939200	2.33269800	2.31567800
H	-7.64380200	-1.27449200	-0.91905300	C	6.03078000	1.39839200	2.48491100

C	7.04796900	-0.87391400	1.67675200	C	-0.57558500	-2.56725400	-4.42529500
C	6.34241000	-1.91621800	0.78267800	H	1.38924500	-2.30969800	-3.64988900
C	5.53688100	-1.06223400	-0.25516700	C	-2.16827300	-3.77776100	-3.06569200
H	4.97314800	3.21331800	2.94974800	C	-1.88003300	-3.10482700	-4.22280400
H	6.77676800	1.54156600	3.26213900	H	-0.35818000	-2.01968200	-5.33837800
H	8.02500000	-0.58674100	1.26473100	H	-3.16069800	-4.18754300	-2.89353800
H	5.63631400	-2.50215000	1.38263500	H	-2.63970600	-2.97940300	-4.98970600
H	7.03226500	-2.61575100	0.30168600	C	3.57673900	3.82364400	-1.03711600
H	7.23179100	-1.24188200	2.69220100	C	2.72712400	3.94825300	0.10940300
C	6.49609200	-0.61152500	-1.40868300	C	3.39693000	4.60394200	-2.14916200
H	7.47373400	-0.29097000	-1.03721200	C	2.88379800	3.15405300	1.27375400
H	6.04395100	0.23700800	-1.93502100	C	1.69197600	4.95719800	0.06579500
C	6.56802800	-1.83291500	-2.35125400	C	2.35752000	5.57707200	-2.19667300
C	5.20621000	-2.46677600	-2.16878100	H	4.05907900	4.48853400	-3.00254600
C	4.55885900	-1.92834300	-1.04374000	C	2.04005000	3.36403100	2.39517700
C	4.58284400	-3.43001500	-2.95544600	C	0.88408700	5.16484600	1.18768000
H	5.09088300	-3.85869800	-3.81512400	C	1.53386300	5.74889600	-1.11599800
C	3.28976100	-3.84115600	-2.63081900	H	2.23803800	6.19371500	-3.08325000
H	2.80010000	-4.60551400	-3.22673500	C	2.12429100	2.58077300	3.59369300
C	2.57741800	-3.26156900	-1.56739300	C	1.04068700	4.40904600	2.35362200
C	3.23577400	-2.28388300	-0.79758900	H	0.13062500	5.94978000	1.16062200
H	7.37149700	-2.52167000	-2.05652700	H	0.75398600	6.50677300	-1.12700200
H	6.76157700	-1.55258700	-3.39246700	C	1.33385400	2.84943400	4.68256700
O	3.05899000	0.78576800	-0.40884000	H	2.83207200	1.76173700	3.63421300
O	2.53021800	-1.65079500	0.23653800	C	0.23723000	4.65797500	3.51186200
P	1.84096400	-0.20584700	-0.02578300	C	0.38474300	3.91210000	4.65051000
O	0.99357700	0.15122100	1.13894200	H	1.43642100	2.24999800	5.58353800
O	1.13648300	-0.25790200	-1.45030800	H	-0.48680000	5.46858900	3.46980000
H	0.15434400	-0.24326700	-1.38215500	H	-0.21579900	4.12660300	5.53053100
C	1.82022600	-4.66256200	0.91722000	H	2.84811400	-4.35819000	0.75917000
C	0.85119500	-4.38253100	-0.10085400	H	4.38428900	3.10158800	-1.01546400
C	1.47731100	-5.30865300	2.07657100	C	-7.22928900	1.19985800	-1.55088300
C	1.17022900	-3.69195800	-1.29752400	C	-7.28092400	1.14438700	-0.15575300
C	-0.49953400	-4.85029800	0.11693200	C	-6.13564000	0.82188900	0.58131400
C	0.13707900	-5.74040900	2.29966800	C	-4.94872100	0.53257300	-0.09068300
H	2.23467500	-5.50734500	2.82947800	C	-4.90486600	0.65491100	-1.49361300
C	0.16571200	-3.46632600	-2.27398200	C	-6.03279200	0.96846000	-2.24096500
C	-1.46938300	-4.64467200	-0.86850100	H	-8.12420000	1.44817700	-2.11345400
C	-0.81809600	-5.52537300	1.33941000	H	-8.20989100	1.36336700	0.36095900
H	-0.11262000	-6.26746600	3.21681700	H	-6.16364000	0.83107000	1.66531900
C	0.40814900	-2.73745700	-3.48484200	H	-5.99379700	1.05261800	-3.32078300
C	-1.17174000	-3.97316400	-2.05749900	C	-2.74048200	0.21871500	-0.90538900
H	-2.47797200	-5.02020300	-0.70830000	C	-3.57576300	0.21611100	0.38858900
H	-1.83707000	-5.87932100	1.47946900	N	-3.58895900	0.43783000	-1.95153900

C	-3.12738600	0.52652500	-3.34696500	H	-4.67241100	3.05097300	0.40837400
H	-2.24492800	-0.11481500	-3.41156400	11			
H	-3.90405500	0.08387900	-3.97694200	C	-5.69111100	0.05753500	-2.54347900
C	-2.80963600	1.94345800	-3.78922600	C	-4.96864900	-0.11707200	-1.35227900
C	-1.65655100	2.58905700	-3.31515500	C	-4.04696100	0.85428800	-0.97558800
C	-3.65006800	2.62240900	-4.67846000	C	-3.91794800	2.06700000	-1.67798300
C	-1.36495200	3.89520300	-3.70907300	C	-4.72298200	2.24165400	-2.81689800
H	-0.97685900	2.05954400	-2.65314500	C	-5.57870800	1.23728600	-3.27278600
C	-3.35617400	3.92798300	-5.07896500	C	-6.50968600	-1.17836200	-2.85025500
H	-4.53361700	2.12611200	-5.07408100	C	-5.91920100	-2.22346800	-1.87588100
C	-2.21669500	4.56790500	-4.59019800	C	-5.43767400	-1.38367500	-0.64507100
H	-0.46632200	4.37987100	-3.33680100	H	-4.64712200	3.17615700	-3.36467700
H	-4.01517400	4.44090100	-5.77374400	H	-6.14962800	1.38241000	-4.18608200
H	-1.98681200	5.58267200	-4.90259300	H	-7.57753900	-1.00794900	-2.65722900
O	-1.52789300	0.04926300	-0.99825900	H	-5.05098900	-2.71049200	-2.33497500
C	-5.16698200	-3.92994400	3.60077200	H	-6.63133700	-3.00527000	-1.59552500
C	-6.03337500	-2.99392900	3.01301900	H	-6.42623900	-1.48475000	-3.89887000
C	-5.55421800	-1.93872100	2.23952200	C	-6.66076200	-1.07622100	0.28580100
C	-4.16875800	-1.79495500	2.04005500	H	-7.56254600	-0.82460300	-0.27993100
C	-3.32647200	-2.77224000	2.63478100	H	-6.41399100	-0.21733400	0.92059100
C	-3.79205400	-3.83192300	3.41136000	C	-6.81403400	-2.33905200	1.15808200
H	-5.57186100	-4.74001900	4.19942300	C	-5.38836000	-2.83164200	1.26629500
H	-7.10467500	-3.09597400	3.15837400	C	-4.57232000	-2.20474100	0.30963300
H	-6.26103700	-1.26020000	1.78449000	C	-4.85784600	-3.74949400	2.16668700
H	-3.10529400	-4.55294800	3.84454500	H	-5.49331800	-4.24132300	2.89823200
C	-1.98021400	-1.37741000	1.50280000	C	-3.49330400	-4.03015400	2.12379800
C	-3.28876400	-0.88607500	1.29346300	H	-3.06846800	-4.75532200	2.81128000
N	-2.01446600	-2.46924300	2.28524000	C	-2.63104000	-3.37322100	1.22879800
H	-1.21088700	-3.05018500	2.49564800	C	-3.19834200	-2.44158300	0.33880200
H	-1.04055400	-0.99390100	1.13125500	H	-7.45698500	-3.08666500	0.67363100
C	-2.99895100	1.96036200	1.24023100	H	-7.25968600	-2.12751100	2.13618900
C	-1.59574500	1.81464500	1.46763300	O	-3.20485000	0.60301100	0.12157100
C	-1.41801900	1.30726800	2.73664600	O	-2.36006500	-1.74523800	-0.54357200
C	-2.69423900	1.23423000	3.31881000	P	-1.86234900	-0.23887600	-0.20132300
O	-3.62069900	1.71993500	2.49387700	O	-1.00996500	0.25088800	-1.31057300
H	-0.81842500	1.98445200	0.73861400	O	-1.23701400	-0.25405900	1.26162900
H	-0.48349900	1.02051400	3.19586200	H	-0.25153600	-0.24196400	1.23239500
C	-3.13973500	0.78186300	4.65975000	C	-1.27844800	-4.80932700	-0.97333200
H	-3.55921400	1.62567100	5.22184800	C	-0.57539700	-4.45332000	0.22326000
H	-3.92600700	0.02433400	4.56738200	C	-0.67883700	-5.53501000	-1.96991700
H	-2.30176700	0.36687700	5.22282800	C	-1.17194900	-3.71083100	1.27332000
C	-3.58639200	3.11997700	0.47959400	C	0.78990600	-4.91243400	0.35766300
H	-3.33037200	4.05596200	0.98814900	C	0.66757500	-5.98111700	-1.83554200
H	-3.16345100	3.15833200	-0.52883600	H	-1.23800100	-5.78842800	-2.86592500

C	-0.41961900	-3.39718200	2.43452400	C	5.52032900	1.38906500	2.77297500
C	1.50633100	-4.62005200	1.52211600	H	7.49316400	2.20780600	3.01876400
C	1.37572500	-5.68407900	-0.69906000	H	7.92489500	2.42418900	0.58752700
H	1.11658600	-6.58064300	-2.62283500	H	6.21871300	1.72315600	-1.05322500
C	-0.94789000	-2.61093500	3.51108200	H	5.31431600	1.34172900	3.83567000
C	0.93948000	-3.87562800	2.56078300	C	2.61164000	0.30979500	0.90385300
H	2.52434400	-4.98955900	1.62791400	C	3.60975500	0.48191900	-0.28256900
H	2.38677600	-6.06295400	-0.55920600	N	3.26583200	0.52820800	2.07042300
C	-0.20705900	-2.35096600	4.63550200	C	2.61441500	0.41991300	3.38803100
H	-1.94921300	-2.20825500	3.42090600	H	1.80683400	-0.30548300	3.26663700
C	1.67586800	-3.58922700	3.75396100	H	3.34473700	-0.01621900	4.07530700
C	1.11898800	-2.85663700	4.76831200	C	2.08823000	1.74065100	3.92006100
H	-0.63437900	-1.75415500	5.43640300	C	0.94697900	2.32870500	3.35299400
H	2.68789800	-3.97773200	3.83965900	C	2.71702000	2.38027800	4.99413700
H	1.68207800	-2.65838300	5.67632000	C	0.45916700	3.54119100	3.84034100
C	-4.28989400	3.52959400	0.85054100	H	0.42300500	1.82601700	2.54493600
C	-3.20457500	3.84084500	-0.03063300	C	2.22822700	3.59277100	5.48607300
C	-4.47437800	4.20893400	2.02646200	H	3.58595800	1.92377500	5.46327500
C	-2.98132800	3.15264700	-1.25059900	C	1.10200000	4.17734000	4.90607700
C	-2.32845600	4.92644100	0.34927800	H	-0.43063500	3.98008900	3.39694700
C	-3.59108000	5.25871100	2.40845200	H	2.72515700	4.07539400	6.32287700
H	-5.30803300	3.95136400	2.67358400	H	0.71923100	5.11885500	5.28980600
C	-1.91314600	3.54044500	-2.09817300	O	1.42167100	0.01505100	0.78272600
C	-1.29254300	5.30800800	-0.50813900	C	6.35727000	-2.96473900	-3.61825200
C	-2.55246100	5.60864000	1.58727100	C	6.77498700	-1.66637200	-3.26080400
H	-3.75688100	5.78875300	3.34211700	C	6.03492600	-0.88081300	-2.38426100
C	-1.61580300	2.87342900	-3.33207200	C	4.83342900	-1.37950600	-1.83658600
C	-1.06992000	4.65402800	-1.72280400	C	4.44572900	-2.70008300	-2.21568800
H	-0.65388300	6.14378300	-0.22919400	C	5.18821400	-3.49668900	-3.09508500
H	-1.88569500	6.42588300	1.85229600	H	6.96008400	-3.55513200	-4.30153400
C	-0.60683100	3.30569100	-4.15442500	H	7.70533000	-1.27747300	-3.66523800
H	-2.20384700	2.00774100	-3.61158400	H	6.40602200	0.09899400	-2.11783800
C	-0.02596300	5.07305400	-2.60905800	H	4.85605300	-4.49739800	-3.35680400
C	0.19575600	4.42835000	-3.79761500	C	2.87987900	-1.91705200	-0.81859800
H	-0.42390300	2.79430600	-5.09638400	C	3.80068900	-0.89064200	-0.93364300
H	0.57357400	5.93521400	-2.32503700	N	3.26227400	-2.98720300	-1.57449600
H	0.97210600	4.77598400	-4.47462800	H	2.73455700	-3.85025300	-1.63943200
H	-2.31028900	-4.49734600	-1.08502500	H	1.96472100	-1.95952500	-0.25120500
H	-4.98371400	2.74500200	0.57223900	C	2.96716200	1.52682100	-1.29651100
C	6.74101500	1.88771700	2.30417200	C	1.77574900	1.00361500	-2.01880500
C	6.98700900	2.00369100	0.93631700	C	2.07684500	0.85163200	-3.33695000
C	6.02801400	1.58670500	0.00372700	C	3.42818900	1.25050900	-3.50567700
C	4.82818300	1.04210200	0.44980400	O	3.96091200	1.67137700	-2.39251800
C	4.57979100	0.99064500	1.83197900	H	0.81251100	0.79316400	-1.55027500

H	1.42554200	0.50237100	-4.12572600	C	-2.08756300	-3.62180600	-1.61842100
C	4.27318800	1.23490400	-4.71948300	C	-1.68531300	-3.50014400	-0.24798100
H	4.87998100	2.14360300	-4.78050700	C	-1.22237000	-3.33676800	-2.64400100
H	4.96507900	0.38253100	-4.64045200	C	-2.56620200	-3.74686500	0.83329500
H	3.66856600	1.12051000	-5.62082800	C	-0.31593400	-3.11923300	0.01404700
C	2.72936600	2.92236100	-0.70780800	C	0.11245100	-2.91719000	-2.37731000
H	2.32293300	3.59349500	-1.46957700	H	-1.55538300	-3.43638200	-3.67430900
H	2.00026500	2.85411800	0.10405600	C	-2.09316800	-3.65738200	2.16542700
H	3.66469100	3.32806500	-0.31750800	C	0.14304500	-3.05301300	1.33422200
13-ts				C	0.55348100	-2.82440300	-1.08411900
C	-8.12159600	-1.20069300	-2.43553600	H	0.77909200	-2.67944900	-3.19962600
C	-7.51471000	-1.55625200	-1.22149100	C	-2.93992000	-3.85609300	3.30419800
C	-7.25852000	-0.57294800	-0.26476800	C	-0.70509800	-3.33403300	2.41020900
C	-7.72983700	0.74421100	-0.44586200	H	1.17462300	-2.76307400	1.52042900
C	-8.39529100	1.04915100	-1.64483200	H	1.57228800	-2.52094200	-0.86036200
C	-8.56660500	0.09961300	-2.65313300	C	-2.44298100	-3.80462900	4.58009000
C	-8.16914600	-2.38922200	-3.37274500	H	-3.99711400	-4.02419100	3.14219000
C	-7.19703000	-3.38350400	-2.69908300	C	-0.22430000	-3.29928100	3.75873900
C	-7.30366800	-3.06589400	-1.16961800	C	-1.06285700	-3.53894100	4.81489300
H	-8.75957000	2.06230800	-1.78947000	H	-3.10998600	-3.95408400	5.42483400
H	-9.04429800	0.37674900	-3.58975900	H	0.83054400	-3.08818600	3.92010400
H	-9.18417200	-2.80649000	-3.43828800	H	-0.68337900	-3.51971400	5.83357400
H	-6.17169600	-3.17905400	-3.02938500	C	-9.14544200	0.61244900	2.12576400
H	-7.41807700	-4.43145000	-2.92646500	C	-8.28438700	1.71383900	1.81412800
H	-7.87017100	-2.13161400	-4.39567600	C	-9.82770200	0.55069200	3.31266700
C	-8.55341100	-3.79626400	-0.57037100	C	-7.56743300	1.80711200	0.59497600
H	-9.42080400	-3.75797100	-1.23727300	C	-8.17857800	2.77454000	2.79078200
H	-8.83016200	-3.30220000	0.36796700	C	-9.70342800	1.58954800	4.27900500
C	-8.06535200	-5.23157700	-0.27627400	H	-10.47175400	-0.29944000	3.52149000
C	-6.60003700	-5.01752500	0.03707800	C	-6.75846600	2.94088200	0.33275900
C	-6.19133100	-3.73891700	-0.37247300	C	-7.38411900	3.88984000	2.51168000
C	-5.70863100	-5.88225400	0.66396100	C	-8.90364000	2.66939400	4.01952300
H	-6.02206300	-6.87555800	0.97592400	H	-10.24902600	1.52183900	5.21651200
C	-4.39997100	-5.45529700	0.89230400	C	-5.98648800	3.08284600	-0.86646100
H	-3.68704200	-6.12532200	1.36440600	C	-6.67766700	4.00357100	1.31100200
C	-3.97605200	-4.15875500	0.55647100	H	-7.31752400	4.69097000	3.24560500
C	-4.90557800	-3.29606500	-0.06175400	H	-8.80546300	3.47449600	4.74431600
H	-8.19605500	-5.88551100	-1.15052300	C	-5.22477600	4.19899000	-1.09965300
H	-8.60825300	-5.70184400	0.55179600	H	-5.98587900	2.27560800	-1.58773800
O	-6.54007600	-0.90189700	0.87255600	C	-5.87171900	5.15251600	1.02991400
O	-4.55023400	-1.98684000	-0.35865400	C	-5.17193000	5.25435800	-0.14342600
P	-4.88503000	-0.83902500	0.80652900	H	-4.64503700	4.26984600	-2.01569000
O	-4.46132100	0.45451300	0.09505100	H	-5.83338300	5.94707400	1.77206500
O	-4.35012500	-1.18186100	2.14840200	H	-4.57149800	6.13785500	-0.34757300

H	-3.09558900	-3.95522200	-1.83908100	C	4.90588900	-1.41838900	-3.90370000
H	-9.25682200	-0.18483900	1.40019000	C	3.17671300	-2.79117900	-4.97871500
C	6.39648200	-2.58012400	3.92727800	C	2.62026500	-5.02450200	-4.09668100
C	6.37746900	-1.83908800	2.73579800	H	2.25230300	-6.94722700	-3.24554100
C	5.60169800	-0.68428100	2.66071400	C	5.63509200	-0.18415700	-3.89615400
C	4.99699800	-0.13948600	3.80948900	C	3.91677600	-1.60593100	-4.94127400
C	5.10162700	-0.87221800	5.00602900	H	2.44190200	-2.93260000	-5.76892100
C	5.75283500	-2.10396400	5.06469100	H	1.87410100	-5.13092100	-4.88034800
C	7.17301600	-3.86640100	3.73969300	C	5.43196400	0.77017800	-4.86047800
C	7.34833400	-3.93519600	2.20538900	H	6.35248300	-0.00592400	-3.10387200
C	7.36789700	-2.43929800	1.74678500	C	3.73170100	-0.58290000	-5.92391500
H	4.63828800	-0.46394100	5.89899400	C	4.47270700	0.56786700	-5.89527600
H	5.76912300	-2.66896700	5.99315500	H	6.00135700	1.69548800	-4.83032800
H	8.14352800	-3.82520500	4.25348900	H	2.98853900	-0.74487900	-6.70106800
H	6.48131600	-4.43148700	1.75455300	H	4.32921100	1.33186800	-6.65488000
H	8.24512200	-4.47995700	1.89400300	C	6.47646500	2.35527000	3.28612700
H	6.64200600	-4.73645600	4.14236400	C	5.09071000	2.37456600	3.64854500
C	8.79677600	-1.83683300	1.98020900	C	7.18668500	3.51384000	3.10167400
H	9.24115000	-2.17045900	2.92275500	C	4.32481500	1.19637800	3.84933600
H	8.71497400	-0.74429700	2.01786600	C	4.47643700	3.66810400	3.85153700
C	9.60559600	-2.25246800	0.73501000	C	6.56605000	4.78458600	3.27295100
C	8.54132500	-2.30762000	-0.33822100	H	8.23780700	3.46398400	2.82998200
C	7.25902500	-2.30128100	0.23333900	C	2.96512000	1.29179500	4.23827100
C	8.70543000	-2.35342100	-1.71806700	C	3.14846100	3.74076300	4.28215800
H	9.69773700	-2.36471500	-2.16160600	C	5.24947800	4.85344800	3.64185700
C	7.57325800	-2.39881500	-2.52887500	H	7.14392700	5.69262700	3.12342900
H	7.68228400	-2.46982100	-3.60692300	C	2.12128900	0.14410700	4.39712700
C	6.27279300	-2.33908600	-1.99714800	C	2.38125800	2.59097500	4.48921900
C	6.14044600	-2.24868900	-0.59817700	H	2.70398300	4.71673100	4.46745700
H	10.07923200	-3.23454000	0.87454500	H	4.76493700	5.81535500	3.79188800
H	10.40911100	-1.54651900	0.49608100	C	0.82322700	0.26504700	4.82221500
O	5.41997200	-0.06456600	1.41494000	H	2.51906900	-0.83245700	4.14763700
O	4.86860000	-2.14467500	-0.02425200	C	1.02606000	2.67332300	4.94288900
P	4.26612200	-0.71006500	0.45786800	C	0.26972900	1.54486600	5.11543000
O	2.93168500	-0.90404100	1.06925500	H	0.20312300	-0.62148800	4.92102200
O	4.38379300	0.27904700	-0.77806800	H	0.61115700	3.65767700	5.14790800
H	3.49395400	0.52181600	-1.16127300	H	-0.75749600	1.61895200	5.46183300
C	4.55775800	-4.72447200	-2.08767100	H	5.30968800	-4.63119800	-1.31278800
C	4.36344700	-3.63820700	-3.00107700	H	6.97433200	1.40081400	3.16440400
C	3.81751300	-5.87436100	-2.17749100	C	0.45279900	6.63005200	-2.60565100
C	5.12392500	-2.44312700	-2.95038300	C	-0.69315300	6.35502400	-1.85648400
C	3.37004900	-3.80762900	-4.03784700	C	-0.92453700	5.06606400	-1.35628200
C	2.83156800	-6.02975100	-3.19280000	C	0.00723700	4.06869800	-1.61502500
H	3.98366000	-6.67959500	-1.46707800	C	1.16390000	4.36724600	-2.34619000

C	1.40627300	5.63619100	-2.86118200	H	-1.21562800	-0.13099100	2.13684300
H	0.61832000	7.63215900	-2.99127400	C	-3.22498700	1.98540200	1.85707000
H	-1.41548400	7.14299900	-1.66467600	H	-3.67677600	2.97559600	1.82655500
H	-1.82207600	4.84372300	-0.78964700	H	-3.80741200	1.29155800	0.93826300
H	2.30947400	5.86076100	-3.41649800	H	-3.49858700	1.36052300	2.70779100
C	1.43196900	2.17166800	-1.74823100	C	1.06261800	3.40150800	1.03952300
C	0.03599200	2.59996400	-1.21798500	H	0.98647700	3.30426400	2.12418900
N	1.98354300	3.21846200	-2.43403600	H	2.07992300	3.12221100	0.74995400
C	3.22400100	3.12456700	-3.20480700	H	0.88468300	4.44071500	0.75807300
H	3.47707200	2.06182300	-3.23980700	14			
H	3.00681400	3.44111300	-4.23167600	C	6.05445700	0.23260500	-1.92286800
C	4.38037600	3.93525900	-2.64496700	C	5.14192800	0.35598300	-0.86369400
C	4.85158000	3.71476200	-1.34356400	C	4.19921000	-0.64848300	-0.65829800
C	5.01968600	4.89186900	-3.44239800	C	4.23293100	-1.84749700	-1.39599100
C	5.92884600	4.44772400	-0.84657300	C	5.21240100	-1.96703800	-2.39676100
H	4.39312300	2.95178800	-0.72157400	C	6.09732200	-0.92812300	-2.68860000
C	6.10332200	5.62335800	-2.94981200	C	6.87598000	1.49644000	-2.06359700
H	4.66967900	5.06523600	-4.45838500	C	6.09765400	2.50038300	-1.18353600
C	6.55612500	5.40559600	-1.64834100	C	5.44523400	1.61923600	-0.06540000
H	6.27954800	4.26423200	0.16515500	H	5.25243600	-2.88818700	-2.97059000
H	6.58766700	6.36303500	-3.58179200	H	6.80944100	-1.03145700	-3.50349900
H	7.39618100	5.97571500	-1.26070300	H	7.90094200	1.35113300	-1.69439500
O	1.95258800	1.06649200	-1.58093200	H	5.30115300	2.96892500	-1.77299200
C	-4.09176600	2.17784500	-4.83807900	H	6.72505300	3.29869700	-0.77477500
C	-3.24764900	3.29457500	-4.67988300	H	6.96140900	1.82622900	-3.10529500
C	-2.20788200	3.29701400	-3.75633400	C	6.50236700	1.33346100	1.05558700
C	-1.98645900	2.16035800	-2.94879400	H	7.49445400	1.11444900	0.64872500
C	-2.82739900	1.02965700	-3.17190300	H	6.17664600	0.45964700	1.63166600
C	-3.88415200	1.02833100	-4.08803800	C	6.46816800	2.58941500	1.95188500
H	-4.90280600	2.21199100	-5.56027400	C	5.03120700	3.04370200	1.81761400
H	-3.40840100	4.17506200	-5.29674800	C	4.40707800	2.39808100	0.73785700
H	-1.57632400	4.17199400	-3.67918400	C	4.33034400	3.94642900	2.61018200
H	-4.51650600	0.15245400	-4.20369000	H	4.81750500	4.45505800	3.43823400
C	-1.32997300	0.44929000	-1.61559000	C	2.98669700	4.19184100	2.32962800
C	-1.04919400	1.77233900	-1.90155400	H	2.43127000	4.90825600	2.92772800
N	-2.37919100	0.00743800	-2.36863000	C	2.30739900	3.50926600	1.30612400
H	-2.88037600	-0.84806000	-2.16534600	C	3.04052700	2.58770900	0.53207100
H	-0.84536500	-0.23522500	-0.94117200	H	7.16560700	3.35846300	1.59077400
C	0.04327700	2.46809900	0.36982700	H	6.74514500	2.37645200	2.99067700
C	0.15740500	1.08328400	0.94049500	O	3.19643600	-0.45256000	0.29550100
C	-0.96983200	0.78260900	1.61172600	O	2.39021700	1.86806000	-0.46960000
C	-1.87680200	1.90279900	1.48078900	P	1.86398600	0.34530100	-0.20216600
O	-1.28989100	2.88819900	0.80979900	O	1.18730900	-0.16287600	-1.41304500
H	1.04471000	0.46652800	0.83828200	O	1.07331400	0.36491900	1.17181800

H	0.10686100	0.16834400	1.04377000	H	-0.11560800	-4.61987500	-4.92277900
C	1.34339700	4.83323000	-1.14685400	H	2.39466700	4.59366600	-1.03783000
C	0.43938900	4.46995400	-0.09660900	H	4.98175200	-2.54247000	0.97052500
C	0.90861900	5.47272100	-2.27853700	C	-6.80195600	-2.16375800	1.90719100
C	0.85677400	3.79992000	1.08074100	C	-7.03151800	-2.16993800	0.53029300
C	-0.95014600	4.83454100	-0.25686400	C	-6.04395100	-1.72230700	-0.35909900
C	-0.46550700	5.81228300	-2.44037900	C	-4.83475000	-1.25947600	0.14632100
H	1.61805300	5.73003100	-3.06018700	C	-4.61100600	-1.29359300	1.53108000
C	-0.08769900	3.48941200	2.09163600	C	-5.57722200	-1.73128000	2.43020100
C	-1.86461500	4.53703800	0.75700900	H	-7.57431400	-2.51375900	2.58656800
C	-1.36383600	5.50814500	-1.45105700	H	-7.98061100	-2.52778500	0.14176900
H	-0.79089200	6.32796200	-3.33998500	H	-6.21020300	-1.73867300	-1.42972700
C	0.26036800	2.78378700	3.29031300	H	-5.38795400	-1.76225000	3.49748500
C	-1.46981400	3.88041700	1.92541800	C	-2.61667200	-0.60378600	0.65192100
H	-2.90813300	4.81702500	0.63100000	C	-3.57838900	-0.75610000	-0.55293100
H	-2.41126700	5.78731800	-1.54477100	N	-3.29567500	-0.86379500	1.80875200
C	-0.67086300	2.52790500	4.26402400	C	-2.69736900	-0.72334700	3.13870800
H	1.27894500	2.43744400	3.41583000	H	-1.90087000	0.01807400	3.03466900
C	-2.41025600	3.59398400	2.96502400	H	-3.45850100	-0.29716100	3.80001400
C	-2.02408300	2.94756800	4.10831600	C	-2.14998100	-2.01597400	3.71853400
H	-0.37627400	1.99376300	5.16355300	C	-0.99858200	-2.60299900	3.17249200
H	-3.44214900	3.90586900	2.82340800	C	-2.76445400	-2.62672500	4.81703500
H	-2.74541600	2.74519900	4.89572900	C	-0.48371500	-3.78343600	3.70773600
C	4.30293500	-3.37429300	1.11906600	H	-0.49667300	-2.12417000	2.33644700
C	3.37484200	-3.70386300	0.07881700	C	-2.25020700	-3.80843500	5.35631400
C	4.35384600	-4.08888300	2.28755900	H	-3.64666900	-2.17174800	5.26295700
C	3.29384200	-2.98346900	-1.13957600	C	-1.11081000	-4.39012400	4.79982600
C	2.51155000	-4.84325200	0.29303200	H	0.41347300	-4.22117800	3.27827200
C	3.48346000	-5.19553900	2.50277400	H	-2.73930400	-4.27060600	6.20980100
H	5.06804900	-3.81289200	3.05869700	H	-0.70804200	-5.30852900	5.21882000
C	2.37985700	-3.38631600	-2.14484400	O	-1.42924500	-0.28274800	0.59029100
C	1.62939400	-5.23817400	-0.71636000	C	-6.50005200	3.69413600	-2.08046100
C	2.59330200	-5.56148100	1.52818900	C	-7.02675700	2.54789800	-1.45511900
H	3.53993900	-5.75264000	3.43415900	C	-6.22070600	1.46810300	-1.11383600
C	2.22859200	-2.68446600	-3.38493900	C	-4.83861400	1.50628800	-1.39432200
C	1.54711400	-4.54851700	-1.92885600	C	-4.33602600	2.68989200	-2.01557200
H	0.99490500	-6.10776000	-0.55635800	C	-5.14366000	3.77645200	-2.36675400
H	1.93603400	-6.41669600	1.66888400	H	-7.15744300	4.51985800	-2.33897400
C	1.36139300	-3.12415600	-4.35091300	H	-8.08969500	2.50489400	-1.23191900
H	2.80112800	-1.77942500	-3.54564600	H	-6.66397500	0.61215000	-0.62343600
C	0.65346200	-4.97217100	-2.96272900	H	-4.71948700	4.65265900	-2.85129200
C	0.56673900	-4.28834100	-4.14499100	C	-2.59534700	1.32160000	-1.65753300
H	1.26877800	-2.57233300	-5.28269700	C	-3.69515100	0.62976000	-1.19016600
H	0.04328600	-5.85473300	-2.78510500	N	-2.97628200	2.53394000	-2.16995700

H	-2.33639900	3.24914200	-2.48486000	H	-6.87443300	-3.37728500	2.24844900
H	-1.55378000	1.04134600	-1.64953200	H	-6.42002400	-2.22905400	3.50287900
C	-3.02259400	-1.86456000	-1.55817500	O	-3.16022600	0.44263600	0.35412200
C	-1.78624600	-1.48111500	-2.33429800	O	-2.24917100	-1.90636300	-0.17403100
C	-2.07318400	-1.47574800	-3.64160300	P	-1.78424800	-0.34564600	-0.02787600
C	-3.48216400	-1.80046000	-3.82995700	O	-1.09170400	0.07083500	-1.26682200
O	-4.03235600	-2.02417800	-2.58482700	O	-1.04768200	-0.19021500	1.36253000
H	-0.82480300	-1.28511500	-1.87420100	H	-0.05248000	-0.11928700	1.27607200
H	-1.38926500	-1.27478200	-4.45673400	C	-1.18231600	-4.84986500	-0.70250400
C	-4.19759100	-1.90664700	-4.95873100	C	-0.22334600	-4.36752100	0.24643000
H	-5.25025300	-2.16362600	-4.94180700	C	-0.79672900	-5.52087400	-1.83379000
H	-3.72619500	-1.72538000	-5.91726300	C	-0.58898800	-3.65837900	1.41875800
C	-2.82263300	-3.22103900	-0.86100900	C	1.17007200	-4.64841400	-0.01397300
H	-2.49238900	-3.95434400	-1.60205900	C	0.58127400	-5.76700800	-2.10062000
H	-2.05037500	-3.15293100	-0.08724400	H	-1.54849600	-5.87454900	-2.53436200
H	-3.75141000	-3.57505600	-0.40654900	C	0.40756600	-3.25088700	2.34116600
15-ts				C	2.13882300	-4.24648100	0.90968800
C	-6.02921900	-0.66233900	-1.67388900	C	1.53363600	-5.34701500	-1.20951300
C	-5.08335400	-0.60705900	-0.63801100	H	0.86850200	-6.30371000	-3.00119300
C	-4.18127500	0.45482400	-0.59819700	C	0.10997200	-2.51657900	3.53606900
C	-4.28383800	1.53576000	-1.49537700	C	1.79402000	-3.56893700	2.08198200
C	-5.29258000	1.47912800	-2.47232300	H	3.18550300	-4.46510000	0.71056400
C	-6.14280200	0.37940100	-2.58875100	H	2.58870100	-5.53686800	-1.39156500
C	-6.80217200	-1.96230300	-1.61869100	C	1.09493900	-2.17415600	4.42679300
C	-5.95235400	-2.81259900	-0.64942300	H	-0.91455700	-2.22143100	3.72804100
C	-5.29930800	-1.77156700	0.32241800	C	2.79135500	-3.18674900	3.03346000
H	-5.38272400	2.30905300	-3.16690200	C	2.45508900	-2.52100300	4.18120300
H	-6.88178200	0.34243700	-3.38520900	H	0.83715300	-1.62571900	5.32925300
H	-7.81844300	-1.80721300	-1.22976700	H	3.82675000	-3.44235700	2.82204000
H	-5.15696300	-3.32246600	-1.20519000	H	3.22085000	-2.24597900	4.90165300
H	-6.52990600	-3.57538700	-0.11807700	C	-4.36290200	3.43114300	0.75548100
H	-6.91123000	-2.42722900	-2.60519900	C	-3.47300100	3.63114600	-0.34889000
C	-6.31848100	-1.40426300	1.45306400	C	-4.42505400	4.32122300	1.79587900
H	-7.33663500	-1.27392500	1.07305900	C	-3.38527700	2.73070500	-1.43983100
H	-6.00884000	-0.45848800	1.91234900	C	-2.65900800	4.82562900	-0.34201900
C	-6.18867100	-2.55042500	2.48087300	C	-3.60398600	5.48500700	1.80814100
C	-4.74328600	-2.97096400	2.32106900	H	-5.10908900	4.14125900	2.62080000
C	-4.19401400	-2.41319700	1.15542400	C	-2.51276500	3.00686700	-2.52168500
C	-3.97270100	-3.77328800	3.15632900	C	-1.81642600	5.09104500	-1.42504400
H	-4.40047500	-4.21644400	4.05211800	C	-2.75058000	5.72827800	0.76479200
C	-2.63728500	-4.00843800	2.82742200	H	-3.66748400	6.18052700	2.64069200
H	-2.03108700	-4.65464000	3.45539600	C	-2.35913300	2.12593400	-3.64176600
C	-2.03189100	-3.40063800	1.71468800	C	-1.72831300	4.22134900	-2.51544000
C	-2.83231000	-2.57086000	0.90463100	H	-1.22019600	6.00147700	-1.42265300

H	-2.13108000	6.62225400	0.75090300	H	6.35143800	-4.40167800	-3.79817400
C	-1.53695300	2.44406200	-4.69167800	H	7.63583200	-2.88662200	-2.31168400
H	-2.89572500	1.18511800	-3.64450600	H	6.51237800	-1.15197100	-0.99106100
C	-0.87959200	4.51334900	-3.62957700	H	3.86974000	-4.19881500	-3.95441300
C	-0.79155300	3.65819300	-4.69424100	C	2.29545800	-1.22758700	-1.55720400
H	-1.44414200	1.75853500	-5.53014700	C	3.53142100	-0.76081700	-1.10440000
H	-0.30447100	5.43611000	-3.60939000	N	2.47400000	-2.25084900	-2.44830400
H	-0.14557200	3.89275500	-5.53588700	H	1.72889600	-2.84084000	-2.78838600
H	-2.23614900	-4.68189200	-0.51325400	H	1.30338200	-0.92102900	-1.27024900
H	-5.00299700	2.55645100	0.76014700	C	3.01637900	2.21800000	-1.39707100
C	6.89259800	2.17407600	1.91355800	C	1.67291500	1.84457800	-1.69483800
C	7.14925300	1.80667500	0.58934600	C	1.67010800	1.24673300	-2.91912700
C	6.16596500	1.17464000	-0.18119000	C	3.00754400	1.34260600	-3.46408100
C	4.92225900	0.88218400	0.38796000	O	3.79354500	1.98141200	-2.50622900
C	4.66868800	1.31594000	1.71439900	H	0.83224100	1.93789500	-1.02393200
C	5.63564500	1.94690900	2.48823700	H	0.81824500	0.81900500	-3.42828100
H	7.66559200	2.66243100	2.50051500	C	3.52413600	0.97113000	-4.64770300
H	8.11809300	2.02272600	0.14763800	H	4.57155100	1.12283500	-4.87860000
H	6.35688500	0.93933900	-1.22203100	H	2.89240200	0.49625900	-5.38824000
H	5.42436800	2.27354700	3.50117800	C	3.44837200	3.37963300	-0.56313500
C	2.70544100	0.42553500	0.95826900	H	3.24694300	4.30807400	-1.11546200
C	3.67957500	0.32581300	-0.15017900	H	2.88844500	3.41397800	0.37460300
N	3.33612300	1.02920000	2.03527900	H	4.51771900	3.34515200	-0.34548000
C	2.68424600	1.24667800	3.32385100	16			
H	1.89283400	0.49510500	3.39004700	C	-1.02331600	-0.02458500	-0.00074600
H	3.41543500	1.02947500	4.10987000	C	-0.57095200	1.32283800	-0.00016300
C	2.10773400	2.64031600	3.51063300	C	0.79969300	1.27461800	0.00015200
C	0.93564500	3.01551200	2.83633000	C	1.18039800	-0.10978700	-0.00009200
C	2.71900800	3.56398400	4.36589300	O	-0.00213100	-0.86470100	-0.00075000
C	0.39747500	4.29163400	3.00551200	H	-1.21147800	2.19404000	-0.00029500
H	0.43635400	2.29700300	2.19204200	H	1.49555500	2.10445100	0.00075000
C	2.18261200	4.84222200	4.53810000	C	2.36853700	-0.73580700	0.00039400
H	3.61766800	3.28029100	4.90967600	H	2.43197900	-1.81957300	0.00024000
C	1.02236200	5.20883900	3.85539900	H	3.28883100	-0.16077700	0.00094100
H	-0.51627500	4.56439600	2.48429500	C	-2.38684100	-0.58610800	0.00023900
H	2.66992500	5.54735200	5.20653400	H	-2.53225600	-1.21024800	0.89221100
H	0.60135300	6.20184100	3.99005400	H	-3.13809000	0.20463300	-0.01675700
O	1.52489400	0.03849700	0.98451900	H	-2.52260400	-1.24192900	-0.86980200
C	5.83108600	-3.63551600	-3.22975500	17			
C	6.55811100	-2.77109100	-2.39117700	C	5.58116100	2.09749200	0.21781900
C	5.92533600	-1.77576500	-1.65234100	C	4.40949600	1.64174400	-0.40362700
C	4.52958100	-1.61580700	-1.74270000	C	3.16154800	2.03352400	0.09086100
C	3.82126300	-2.52814800	-2.57540200	C	3.08123700	3.00172700	1.11599100
C	4.44811400	-3.52695500	-3.32520300	C	4.27534300	3.48316600	1.67699200

C	5.52332600	3.01751400	1.26031500	H	1.62474800	-6.80349100	1.73766400
C	6.79822800	1.43379100	-0.39166400	C	-1.69288900	-2.92265800	-2.87963900
C	6.17422300	0.27009500	-1.19285800	H	0.16740100	-1.90559400	-3.08255200
C	4.76075000	0.79149800	-1.62095300	C	-1.80384100	-4.74408100	-1.29314300
H	4.21124700	4.22231300	2.47126900	C	-2.42540700	-3.94940700	-2.21729300
H	6.43093400	3.37266400	1.74339200	H	-2.20392200	-2.26963000	-3.58180900
H	7.34437100	2.12496400	-1.05092300	H	-2.35743200	-5.50683700	-0.75158400
H	6.03889500	-0.59728400	-0.53672300	H	-3.48361100	-4.07817700	-2.42923700
H	6.78107300	-0.04710200	-2.04790800	C	1.47160900	4.78297700	-0.56767500
H	7.51422100	1.09107200	0.36539800	C	1.05033400	4.44840400	0.75996000
C	4.89131100	1.66238100	-2.91548600	C	0.75497500	5.65034600	-1.35041100
H	5.76503900	2.32304100	-2.89208600	C	1.77751100	3.56236100	1.59352700
H	3.99734600	2.29045800	-3.00294300	C	-0.15522200	5.07326100	1.25553500
C	4.92322400	0.64078600	-4.07479700	C	-0.43912600	6.25360100	-0.86090300
C	4.08947500	-0.49979300	-3.52823000	H	1.09720800	5.88010100	-2.35625000
C	3.89069600	-0.34406800	-2.14903000	C	1.31913600	3.29115300	2.90530400
C	3.54014500	-1.58351200	-4.20726200	C	-0.58078800	4.80934900	2.56034400
H	3.69464100	-1.70957300	-5.27667200	C	-0.87648100	5.97082200	0.40606800
C	2.78847900	-2.51658500	-3.49007600	H	-0.99485600	6.94110300	-1.49400200
H	2.37614300	-3.38446300	-3.99799400	C	1.98938200	2.37603200	3.78067900
C	2.51736200	-2.35373200	-2.12193400	C	0.12533200	3.94150400	3.39763900
C	3.04517600	-1.22090900	-1.46468900	H	-1.48323400	5.29094500	2.93265900
H	5.95206300	0.31790100	-4.29320400	H	-1.78262800	6.42964000	0.79617800
H	4.51815000	1.04942500	-5.00871400	C	1.54105500	2.15731600	5.05684300
O	2.02166600	1.47930400	-0.43324600	H	2.83820900	1.82389700	3.39898600
O	2.75230500	-0.98527500	-0.14477300	C	-0.30868600	3.68344400	4.73640800
P	1.46972200	0.03190200	0.23357000	C	0.38216500	2.82502300	5.54799100
O	1.48384600	0.11378700	1.72752700	H	2.05963500	1.44749600	5.69610200
O	0.27472800	-0.31781700	-0.60090300	H	-1.20804700	4.18264100	5.09051800
H	-1.43129300	-0.18085400	-0.83499300	H	0.03910100	2.63296600	6.56170100
C	3.74539500	-4.13391900	-0.14077800	H	4.34487300	-3.39609600	-0.66193200
C	2.34773200	-4.22090500	-0.44174700	H	2.37925900	4.33330400	-0.95317500
C	4.33310600	-4.95967800	0.78223900	C	-7.90647000	-0.86607400	0.05197400
C	1.71292500	-3.38111700	-1.39017500	C	-7.42014900	-1.43722200	1.24034800
C	1.57783600	-5.22842300	0.25160600	C	-6.05198500	-1.50062900	1.50338200
C	3.56414100	-5.93587000	1.47836400	C	-5.14360800	-0.99281600	0.56079600
H	5.39646000	-4.86735500	0.99010600	C	-5.66067600	-0.41142800	-0.63445300
C	0.33727500	-3.55010500	-1.67642000	C	-7.02745600	-0.34019800	-0.89857200
C	0.21937000	-5.37822200	-0.04006000	H	-8.97785600	-0.82334200	-0.12943700
C	2.22638000	-6.06252700	1.21579800	H	-8.12372000	-1.83116500	1.97070900
H	4.04370700	-6.57642000	2.21474800	H	-5.68578300	-1.93573600	2.42915100
C	-0.36404600	-2.72352200	-2.61262000	H	-7.40385800	0.12198900	-1.80743900
C	-0.41601000	-4.57592000	-0.99084600	C	-3.41179900	-0.26968800	-0.68870700
H	-0.36095800	-6.12617400	0.49555400	C	-3.70545600	-0.89095000	0.51611900

N	-4.57894900	0.01926700	-1.38935100	H	5.11996000	-3.31356800	1.21424200
C	-4.62736100	0.67485500	-2.68585300	H	6.51280800	-3.54775300	0.14874500
H	-3.68215300	0.44847500	-3.18721700	H	6.84647000	-2.42150600	2.65113400
H	-5.43325500	0.21539000	-3.26989400	C	6.30954500	-1.37160100	-1.41248700
C	-4.82852500	2.18230600	-2.62294700	H	7.32135900	-1.23510500	-1.01783200
C	-3.84917300	3.00088300	-2.04087700	H	5.99984500	-0.42728300	-1.87465000
C	-5.97714100	2.77707700	-3.15478400	C	6.20262300	-2.51784200	-2.44392900
C	-4.02325300	4.38328800	-1.98873400	C	4.75891200	-2.95204200	-2.30374000
H	-2.95047800	2.54621300	-1.63338000	C	4.18870600	-2.39507900	-1.14811900
C	-6.15358800	4.16265700	-3.10554000	C	4.00615300	-3.76546100	-3.14494700
H	-6.74176500	2.15170400	-3.61218600	H	4.44978200	-4.20999000	-4.03232200
C	-5.17665000	4.96859600	-2.52046700	C	2.66783200	-4.01047400	-2.83355200
H	-3.25158300	5.00036900	-1.53559500	H	2.07665700	-4.66570700	-3.46647700
H	-7.05458900	4.60852200	-3.52074200	C	2.04117200	-3.39976800	-1.73418300
H	-5.31151700	6.04696400	-2.47886600	C	2.82483100	-2.55994100	-0.91810000
O	-2.27615000	0.10195200	-1.28703600	H	6.89331700	-3.33854400	-2.20454200
C	-1.60745100	-4.79285300	3.63131700	H	6.44378200	-2.19223400	-3.46233200
C	-2.81822800	-4.87419100	2.91310900	O	3.13308900	0.46333300	-0.35239300
C	-3.29058200	-3.79040100	2.17773900	O	2.22125800	-1.89204000	0.14554900
C	-2.54868400	-2.59704200	2.15675400	P	1.75088700	-0.33430600	-0.01728300
C	-1.32605800	-2.53459900	2.89383800	O	1.02100500	0.06660300	1.20553200
C	-0.84971300	-3.62460300	3.62963200	O	1.05473800	-0.17382400	-1.42475600
H	-1.25932400	-5.65486400	4.19638200	H	0.04911700	-0.15348600	-1.37568300
H	-3.39036200	-5.79952900	2.93479600	C	1.15605500	-4.79310900	0.70440200
H	-4.21940800	-3.86391600	1.61852100	C	0.21083600	-4.32534000	-0.26522700
H	0.08805900	-3.56111900	4.17604300	C	0.75332300	-5.42270500	1.85351900
C	-1.62048200	-0.56672600	1.87884200	C	0.59444500	-3.65337600	-1.45423000
C	-2.70878300	-1.31697900	1.49873900	C	-1.18807200	-4.57990200	-0.00686400
N	-0.79638600	-1.27297700	2.72406200	C	-0.62992700	-5.63745400	2.11964800
H	0.18149500	-0.99490100	2.80218300	H	1.49549700	-5.76715300	2.56881900
H	-1.34871200	0.43617300	1.58858300	C	-0.38980300	-3.26449900	-2.39783200
18-ts				C	-2.14379100	-4.19847700	-0.95278400
C	5.96227100	-0.65482600	1.72463600	C	-1.56986600	-5.23209100	1.20891000
C	5.03807500	-0.59284500	0.66946800	H	-0.93142600	-6.14006800	3.03514600
C	4.13075600	0.46493700	0.62441500	C	-0.07552300	-2.56510600	-3.60921500
C	4.20507900	1.53198500	1.54081800	C	-1.78137700	-3.56341700	-2.14322600
C	5.18990600	1.46722800	2.54086400	H	-3.19458300	-4.39959600	-0.75652000
C	6.04683600	0.37284000	2.65830500	H	-2.62869700	-5.40012500	1.39067700
C	6.74800300	-1.94680400	1.66817800	C	-1.04931500	-2.23940400	-4.51813500
C	5.92130700	-2.79343000	0.67676200	H	0.95282700	-2.28251400	-3.79974300
C	5.27730500	-1.74838800	-0.29741200	C	-2.76620400	-3.20249600	-3.11565100
H	5.25614500	2.28627200	3.25096900	C	-2.41402900	-2.57016000	-4.27724800
H	6.76806000	0.32837000	3.47050800	H	-0.77892200	-1.71630100	-5.43185200
H	7.76850100	-1.77789400	1.29634600	H	-3.80567300	-3.44386000	-2.90758500

H	-3.17077400	-2.30837700	-5.01194500	C	-0.38170200	4.34273400	-2.73710500
C	4.38807300	3.50025200	-0.63591600	H	-0.46180900	2.31629900	-2.01015300
C	3.44261300	3.66158300	0.42778700	C	-1.99724900	4.91785600	-4.43908300
C	4.50371900	4.42823400	-1.63809800	H	-3.34420600	3.34298300	-5.02625100
C	3.30209300	2.72403500	1.48084100	C	-0.92971400	5.28046300	-3.61757500
C	2.62645400	4.85466000	0.42087100	H	0.46393600	4.61155000	-2.11002400
C	3.68518000	5.59357600	-1.64891000	H	-2.42407000	5.63871600	-5.13176700
H	5.22849700	4.27705500	-2.43350200	H	-0.51931900	6.28569800	-3.66803000
C	2.37188600	2.95803400	2.52309100	O	-1.51928100	-0.15888600	-1.13321300
C	1.72049200	5.07497100	1.46241100	C	-5.68471400	-3.43748900	3.51615700
C	2.77753500	5.79884700	-0.64402700	C	-6.45867400	-2.73342000	2.57481000
H	3.79159400	6.31927400	-2.45070400	C	-5.87110800	-1.82223300	1.70361600
C	2.16912300	2.03989400	3.60447800	C	-4.48469700	-1.59239800	1.76483900
C	1.57565900	4.16473700	2.51285200	C	-3.72499800	-2.33752700	2.70910500
H	1.11844600	5.98160400	1.45880000	C	-4.30858400	-3.25258400	3.59165800
H	2.15775300	6.69270600	-0.62976000	H	-6.16638700	-4.14424400	4.18671000
C	1.27994300	2.31036600	4.61192600	H	-7.52894400	-2.91146000	2.52128300
H	2.72112500	1.10801600	3.60899900	H	-6.47956200	-1.32222900	0.96065000
C	0.65659900	4.40666400	3.58238800	H	-3.70268800	-3.80641900	4.30376000
C	0.51523800	3.51229800	4.60837700	C	-2.24859700	-1.10963200	1.51267100
H	1.14690500	1.59587600	5.42010800	C	-3.54380300	-0.81849800	0.96626100
H	0.07122900	5.32293200	3.55941900	N	-2.38935800	-2.03532700	2.53064600
H	-0.18615400	3.70685800	5.41510500	H	-1.62919100	-2.60691700	2.86856200
H	2.21358000	-4.64835300	0.51658500	H	-1.30715800	-1.01180000	0.99882300
H	5.02637900	2.62404100	-0.64045000	C	-3.01860100	2.45005200	1.68127000
C	-6.76542100	2.24914900	-2.12428200	C	-1.79360000	1.84557000	1.57193100
C	-7.10171600	1.77111000	-0.85418300	C	-1.73347200	0.83424600	2.55997000
C	-6.18816400	1.02301500	-0.10270200	C	-2.90794000	1.02150500	3.38895000
C	-4.92607500	0.72332500	-0.63524300	O	-3.72323800	1.95844600	2.74654500
C	-4.59054500	1.27365100	-1.90473100	H	-1.04008300	2.05504700	0.82869400
C	-5.49052300	2.01877400	-2.65676200	H	-0.81933900	0.37186400	2.90062000
H	-7.48670800	2.82598700	-2.69651100	C	-3.27747100	0.48729600	4.56497100
H	-8.08106400	1.98990600	-0.43718300	H	-4.22358200	0.74397000	5.02660600
H	-6.45099400	0.70431800	0.89926500	H	-2.62812100	-0.21840000	5.06665500
H	-5.21002500	2.43329900	-3.61939000	C	-3.65886900	3.56043100	0.93430200
C	-2.70054900	0.24989500	-1.13388400	H	-3.80090900	4.43187400	1.58667000
C	-3.74555200	0.04398400	-0.13181600	H	-3.04014200	3.85138900	0.08203000
N	-3.26031900	0.95973600	-2.19077200	H	-4.64666400	3.25744700	0.56714600
C	-2.54312100	1.26730000	-3.42213600	19			
H	-1.73389000	0.53468700	-3.48721100	C	-6.01804900	-0.71056800	-1.61002100
H	-3.22175100	1.08846200	-4.26383100	C	-5.07048900	-0.65501000	-0.57543300
C	-1.98526800	2.67951700	-3.49062500	C	-4.17366500	0.41180200	-0.53583100
C	-0.90558000	3.05143300	-2.67591900	C	-4.27835200	1.49177700	-1.43368600
C	-2.51884300	3.62321300	-4.37471800	C	-5.28506900	1.43158400	-2.41186100

C	-6.13372900	0.33015500	-2.52582500	H	2.68641900	-5.24794000	-1.52380600
C	-6.78723500	-2.01272400	-1.55678000	C	1.13244900	-2.20682100	4.45632000
C	-5.92749400	-2.86593500	-0.59940900	H	-0.88304000	-2.31816600	3.78442200
C	-5.27393800	-1.82954000	0.37739900	C	2.85045200	-3.08889600	3.00231200
H	-5.37474500	2.25958800	-3.10888200	C	2.50252000	-2.48376900	4.17977600
H	-6.87211500	0.28997200	-3.32269000	H	0.86428200	-1.70453100	5.38223200
H	-7.80072300	-1.86278600	-1.15852600	H	3.89296000	-3.29024200	2.76825100
H	-5.13268900	-3.36669800	-1.16423800	H	3.26611500	-2.20392900	4.90065700
H	-6.49758400	-3.63629900	-0.07087200	C	-4.43329600	3.42871800	0.77279800
H	-6.90295600	-2.47234700	-2.54499300	C	-3.50980800	3.61148500	-0.30667300
C	-6.28492600	-1.48370000	1.52193900	C	-4.53442100	4.34054100	1.79140400
H	-7.30757900	-1.35615600	1.15317700	C	-3.38259200	2.68981900	-1.37542400
H	-5.97793800	-0.54166900	1.99052600	C	-2.70102600	4.80953900	-0.29779900
C	-6.13796000	-2.64270900	2.53412100	C	-3.72240400	5.51040100	1.80411600
C	-4.69105100	-3.05172000	2.35622500	H	-5.24284100	4.17298600	2.59825900
C	-4.15749800	-2.47377100	1.19340400	C	-2.47152400	2.94310300	-2.43007800
C	-3.90480100	-3.85843000	3.17303300	C	-1.81736400	5.05106300	-1.35362500
H	-4.32058100	-4.31928700	4.06554400	C	-2.83639200	5.73630300	0.78434400
C	-2.56810400	-4.07289700	2.83262600	H	-3.81703300	6.22330500	2.61881500
H	-1.95026900	-4.71966600	3.44868000	C	-2.27705000	2.03789900	-3.52364500
C	-1.97802300	-3.44080200	1.72539800	C	-1.68428400	4.15569900	-2.41814800
C	-2.79697100	-2.61387500	0.93063900	H	-1.22139100	5.96172500	-1.34858900
H	-6.82054400	-3.47094500	2.29734400	H	-2.22282600	6.63453600	0.77092500
H	-6.36205700	-2.33585400	3.56218500	C	-1.40271300	2.32500100	-4.53933700
O	-3.14888800	0.40350700	0.41367000	H	-2.82009000	1.10085500	-3.52925100
O	-2.23107300	-1.93285400	-0.14432200	C	-0.78331200	4.41669800	-3.49824200
P	-1.77161400	-0.37205000	0.01443700	C	-0.64772300	3.53304100	-4.53412600
O	-1.08455100	0.05145300	-1.22330900	H	-1.27248100	1.61845700	-5.35477400
O	-1.02622600	-0.22871200	1.40356900	H	-0.20422900	5.33689300	-3.47358100
H	-0.03690000	-0.13301500	1.30798400	H	0.04310000	3.73965900	-5.34680300
C	-1.10063100	-4.79175400	-0.73910500	H	-2.15784600	-4.68877400	-0.52400300
C	-0.14999000	-4.29692600	0.21150100	H	-5.06674600	2.54886900	0.77624100
C	-0.70253300	-5.39548200	-1.90342700	C	6.96951000	1.91612900	2.19090700
C	-0.53028300	-3.65003100	1.41522000	C	7.30100800	1.45112600	0.91562400
C	1.25092500	-4.49491300	-0.08332700	C	6.34353400	0.81974900	0.11444600
C	0.68076400	-5.55463000	-2.20481100	C	5.04844400	0.62644300	0.60520500
H	-1.44828800	-5.76100400	-2.60429500	C	4.72279600	1.15727300	1.87953200
C	0.46122600	-3.23410000	2.33996300	C	5.66397000	1.79004100	2.68223400
C	2.21453900	-4.08504200	0.84264900	H	7.72310200	2.40382100	2.80304400
C	1.62722500	-5.12194200	-1.31396900	H	8.30854700	1.59096800	0.53435700
H	0.97826700	-6.03588300	-3.13292200	H	6.60318300	0.50993900	-0.89158600
C	0.15034200	-2.55915300	3.56631300	H	5.39679200	2.19654000	3.65176500
C	1.85693200	-3.47713000	2.04899600	C	2.75426900	0.37481700	1.01893600
H	3.26716300	-4.24478700	0.61936100	C	3.81661900	0.09835000	0.02574900

N	3.35750400	0.95929500	2.11903800	H	4.18676700	1.24080200	-5.15377100
C	2.63753900	1.27070600	3.35211200	20-ts			
H	1.80983300	0.55855800	3.40563900	C	5.88051200	-2.24119400	1.12494700
H	3.31017100	1.06086000	4.19037600	C	4.82293400	-1.97240200	0.24241300
C	2.11719900	2.69595200	3.43519500	C	4.29984400	-0.68273800	0.17451700
C	0.98548600	3.07723800	2.69904800	C	4.92624100	0.39129900	0.83705100
C	2.73869700	3.64315500	4.25629100	C	6.04521800	0.09826300	1.63667800
C	0.49650700	4.38167000	2.77430700	C	6.49919800	-1.20803700	1.82110300
H	0.47914400	2.34264800	2.07961900	C	6.16813400	-3.72770300	1.17025200
C	2.25291600	4.95066400	4.33317800	C	4.94573000	-4.32970900	0.43869800
H	3.60429900	3.35643300	4.84987500	C	4.51395700	-3.21998400	-0.57577600
C	1.13258800	5.32256600	3.58954000	H	6.54164200	0.91882400	2.14592900
H	-0.38995600	4.65726300	2.20936000	H	7.32957800	-1.40747500	2.49389400
H	2.74743200	5.67406300	4.97631100	H	7.10608700	-3.97238500	0.65242000
H	0.74982200	6.33799000	3.65132700	H	4.12921100	-4.49298100	1.15142500
O	1.54975600	0.07365900	0.98198000	H	5.15947500	-5.28533600	-0.05076600
C	5.46331700	-3.69430200	-3.34712300	H	6.27078900	-4.10052600	2.19593900
C	6.27139600	-3.04974200	-2.39088000	C	5.44007600	-3.28089400	-1.83965800
C	5.76447600	-2.00341600	-1.63089400	H	6.48610900	-3.47164500	-1.58117900
C	4.43635800	-1.57652600	-1.82469100	H	5.39430100	-2.31437100	-2.35466900
C	3.63096700	-2.25516600	-2.78355800	C	4.81505900	-4.37280500	-2.73042000
C	4.14257000	-3.31297700	-3.55100400	C	3.34565200	-4.26180800	-2.39054600
H	5.87784000	-4.50966300	-3.93449900	C	3.16133200	-3.51379400	-1.21656500
H	7.29570100	-3.37814700	-2.24230000	C	2.25832400	-4.77522600	-3.08863900
H	6.38361800	-1.54093100	-0.87260200	H	2.40272500	-5.36160500	-3.99258500
H	3.51725700	-3.81697000	-4.28227600	C	0.97359000	-4.52415500	-2.61196600
C	2.22307700	-0.69812900	-1.79356400	H	0.11295700	-4.92954800	-3.13575200
C	3.57594000	-0.66559600	-1.10035000	C	0.74503500	-3.72835300	-1.47590900
N	2.35878300	-1.74763900	-2.80096300	C	1.86493200	-3.20709900	-0.79805300
H	1.57158900	-2.35282200	-2.99408100	H	5.20765500	-5.36847100	-2.47900700
H	1.39698800	-0.90129700	-1.11113600	H	5.01329100	-4.21641100	-3.79694700
C	2.95562600	1.19933700	-3.44483700	O	3.12746000	-0.46039000	-0.55359600
C	1.86848700	0.68355900	-2.51210300	O	1.68023300	-2.40346800	0.32507100
C	1.71674000	1.85158200	-1.58267600	P	1.72723500	-0.76906600	0.23173600
C	2.67082500	2.74937100	-1.85006900	O	1.59014500	-0.20074900	1.58758600
O	3.48069300	2.37449400	-2.91508500	O	0.71779500	-0.33438900	-0.90259300
H	0.93994300	0.46963600	-3.05048300	H	-0.16665900	0.02087600	-0.56247200
H	0.95651500	1.92466700	-0.82205300	C	-0.35341000	-4.88339000	1.00911000
C	3.02022200	4.05700600	-1.23203600	C	-1.17588100	-4.12255400	0.11671300
H	2.35502100	4.27075000	-0.39156000	C	-0.87267600	-5.47885500	2.12936700
H	4.05416700	4.04425600	-0.86575300	C	-0.67229900	-3.50151000	-1.05284100
H	2.94313900	4.87032000	-1.96447000	C	-2.58455700	-4.02427000	0.42590700
C	3.39805700	0.73010300	-4.61160300	C	-2.25984100	-5.36992600	2.43525100
H	2.98592100	-0.17977100	-5.02755000	H	-0.22261600	-6.04604800	2.79014000

C	-1.54184700	-2.76953000	-1.89946100	C	-4.09909700	3.31214200	-3.06381000
C	-3.43334600	-3.32191800	-0.43450300	H	-5.72467200	4.41301500	-3.94583100
C	-3.08883800	-4.66702300	1.60147200	H	-7.40921700	3.62754500	-2.30233000
H	-2.65538600	-5.85888000	3.32187400	H	-6.76947400	2.09080800	-0.48561400
C	-1.08668600	-2.08618000	-3.07461500	H	-3.35208900	3.69929100	-3.74832600
C	-2.94936600	-2.68835200	-1.58211700	C	-2.57467400	1.13245700	-0.58743700
H	-4.49404400	-3.26170900	-0.20283700	C	-3.99489700	1.05513100	-0.19452700
H	-4.15530000	-4.59597100	1.80504500	N	-2.49419400	1.92393400	-1.72249900
C	-1.95745800	-1.40050100	-3.88174200	C	-1.23816800	2.31380100	-2.35962500
H	-0.02994700	-2.10278600	-3.31229100	H	-0.51317900	1.52768400	-2.13977600
C	-3.82404600	-1.96270300	-2.45116200	H	-1.39441200	2.31560900	-3.44340900
C	-3.34698600	-1.33950500	-3.57272800	C	-0.71774700	3.66452200	-1.89561500
H	-1.58369800	-0.89000700	-4.76565000	C	-0.31449500	3.84400400	-0.56351200
H	-4.87822800	-1.91096600	-2.19138700	C	-0.62899000	4.74337600	-2.78115900
H	-4.02021500	-0.78629800	-4.22166100	C	0.14853500	5.08571700	-0.12845400
C	5.00675800	1.80953800	-1.74548300	H	-0.35843400	3.01038500	0.13215600
C	4.54696900	2.46025800	-0.55528300	C	-0.16075800	5.98661000	-2.34804500
C	5.06402800	2.46846500	-2.94590900	H	-0.92454900	4.61209500	-3.82023400
C	4.47182000	1.80909600	0.70270100	C	0.22333700	6.16155200	-1.01845800
C	4.17990100	3.85418500	-0.66057800	H	0.46058700	5.20636300	0.90516000
C	4.66748000	3.83216400	-3.04868400	H	-0.10149600	6.81581100	-3.04842100
H	5.41702000	1.94608600	-3.83121600	H	0.58142400	7.12958100	-0.67709000
C	4.05834100	2.52946100	1.85169300	O	-1.59091200	0.57572800	-0.05332500
C	3.79514000	4.55353500	0.48631300	C	-7.84215200	-2.18573000	1.82234100
C	4.24244000	4.50247800	-1.93394500	C	-8.01857800	-1.30029300	0.74450200
H	4.71085300	4.33569300	-4.01071500	C	-6.98202200	-0.47473700	0.31852600
C	3.93827700	1.92818200	3.14713200	C	-5.73809100	-0.51460400	0.97461700
C	3.73713600	3.93461300	1.73748400	C	-5.57514900	-1.45850900	2.03063600
H	3.54054600	5.60786400	0.40242700	C	-6.61749000	-2.27904600	2.47561500
H	3.94192600	5.54568500	-1.99320600	H	-8.66789900	-2.81533700	2.14244500
C	3.59165500	2.66742700	4.24867500	H	-8.97572200	-1.26309700	0.23242400
H	4.11077200	0.86363800	3.24713900	H	-7.13345100	0.16951700	-0.53738900
C	3.37088100	4.66769600	2.91037500	H	-6.46803200	-2.97535400	3.29657400
C	3.31224200	4.05972900	4.13559600	C	-3.57015200	-0.43198000	1.76669100
H	3.51524500	2.18390300	5.21905400	C	-4.43744500	0.11350200	0.75297000
H	3.14672800	5.72685800	2.80476600	N	-4.26746900	-1.41861500	2.45510600
H	3.04331500	4.63036200	5.02066200	H	-3.83151500	-2.09642200	3.06063000
H	0.70247100	-4.98643700	0.78738300	H	-2.50115100	-0.51491800	1.65442100
H	5.32178200	0.77426400	-1.68912600	C	-2.84478200	2.26076000	2.47620200
C	-5.43437700	3.72140200	-3.15985600	C	-3.41065000	1.16569600	3.21797200
C	-6.38437400	3.27257900	-2.23854000	C	-2.35307600	0.73153600	4.09773000
C	-6.02845200	2.38144300	-1.22081600	C	-1.22322500	1.39890000	3.73603000
C	-4.71284400	1.91065300	-1.13407300	O	-1.48348900	2.31137100	2.74675100
C	-3.75725900	2.42379600	-2.05095900	H	-4.46574400	1.11620900	3.45443900

H	-2.41349300	-0.03513800	4.85787000	H	-1.69496300	4.98743300	-2.08042300
C	0.18900600	1.30598600	4.17895300	H	-1.03961200	2.60528100	-2.09101000
H	0.26461000	0.67323500	5.06788200	H	-1.90154700	5.00643900	2.22837500
H	0.80584800	0.87273200	3.38163300	C	-0.87058100	1.00662200	1.81856000
H	0.59184000	2.29829900	4.40962000	C	-0.83935600	1.04063500	0.44396600
C	-3.39912000	3.09736600	1.56719800	N	-1.19905000	2.24798200	2.31776100
H	-4.47096600	3.12561100	1.43556100	H	-0.68319400	0.18006900	2.48711900
H	-2.80040900	3.84238300	1.05577700	H	-1.28446100	2.47558100	3.29569800
3-R				C	-1.74048500	-0.42309900	-1.46250000
C	1.14718600	-3.59282700	1.43689400	H	-1.43483500	-1.22316400	-2.14554300
C	-0.17369700	-3.29774900	1.77603100	H	-1.87331300	0.48003300	-2.06449400
C	-0.82146200	-2.18921100	1.20900800	C	-3.03358800	-0.81528300	-0.83183600
C	-0.13394300	-1.38979700	0.30472200	C	-4.00951900	-0.14090600	-0.15687400
C	1.19180300	-1.70964800	-0.03353300	O	-3.36678900	-2.14804600	-0.90054900
C	1.85320700	-2.79997700	0.52282100	C	-4.99842500	-1.11109800	0.21372800
H	1.64191700	-4.44975100	1.88618400	H	-4.02002800	0.92026200	0.04827900
H	-0.70535800	-3.92797400	2.48320400	C	-4.56578900	-2.31502900	-0.26156500
H	-1.84879100	-1.96051300	1.47460800	H	-5.91791000	-0.93349700	0.75521800
H	2.88407200	-3.02478200	0.27094000	C	-5.12414600	-3.69576200	-0.23431300
C	0.70331900	0.13210300	-1.32372200	H	-6.07073200	-3.70291600	0.31361400
C	-0.55934200	-0.14761500	-0.46095000	H	-5.31328700	-4.07549400	-1.24651700
N	1.67252300	-0.79685000	-0.98678600	H	-4.43935300	-4.39991500	0.25501800
C	2.97786100	-0.84055200	-1.63314900	21-ts			
H	3.16273600	-1.86161800	-1.98791200	C	-5.52026600	2.76390100	-0.52981000
H	2.88516700	-0.19090300	-2.50947100	C	-4.64361800	1.88251700	0.12137500
C	4.12181600	-0.37765100	-0.74735800	C	-3.29378300	2.21553400	0.22899800
C	5.23920300	-1.19241700	-0.53877600	C	-2.82049000	3.47674600	-0.18236200
C	4.08497400	0.89046800	-0.15066500	C	-3.74653100	4.36404000	-0.75955000
C	6.30315500	-0.75478500	0.25445700	C	-5.07900500	4.00882200	-0.96616800
H	5.28130900	-2.17564200	-1.00358800	C	-6.89339400	2.14262700	-0.66868500
C	5.14369500	1.32756200	0.64398200	C	-6.62194900	0.65914000	-0.33574000
H	3.22549500	1.53509500	-0.31597800	C	-5.42411700	0.69458800	0.67331000
C	6.25599600	0.50580200	0.84961800	H	-3.39357900	5.34158700	-1.07442300
H	7.16402400	-1.40016200	0.40811800	H	-5.75811000	4.69918400	-1.46012200
H	5.10343900	2.31315600	1.10022100	H	-7.60730900	2.58804400	0.03844900
H	7.08064300	0.84856600	1.46885800	H	-6.30393000	0.12930400	-1.24110700
O	0.83518400	0.99539000	-2.17654500	H	-7.49451500	0.13637100	0.06825800
C	-1.84864200	5.13315900	0.06888200	H	-7.31602700	2.28084500	-1.67045600
C	-1.61387800	4.44810800	-1.14058100	C	-5.96457400	0.99280300	2.11293000
C	-1.26766800	3.10267400	-1.15590000	H	-6.74236300	1.76279500	2.11595000
C	-1.15884700	2.40567200	0.06448400	H	-5.13518300	1.35247100	2.73273200
C	-1.38803500	3.12662400	1.27088400	C	-6.45145600	-0.37534400	2.63657400
C	-1.73270900	4.48254700	1.29081900	C	-5.52759600	-1.34271300	1.92886000
H	-2.11550600	6.18631500	0.04659900	C	-4.83956000	-0.69848700	0.88791200

C	-5.30811900	-2.68862300	2.20162800	C	1.19396900	5.03072300	0.26840600
H	-5.84961600	-3.19046000	2.99957700	C	1.00915000	4.88938700	2.71945000
C	-4.38309600	-3.39248100	1.43124700	H	0.69476600	4.77112500	4.82882900
H	-4.22051500	-4.45048900	1.61439100	C	-1.09534000	3.99482700	-2.50361600
C	-3.61949500	-2.76406600	0.43263500	C	0.67204200	4.84128300	-1.01406300
C	-3.84517200	-1.39293200	0.19976500	H	2.18542700	5.46448600	0.37989800
H	-7.50158900	-0.55682600	2.36772200	H	2.01674500	5.28987800	2.80104600
H	-6.38782100	-0.45793100	3.72762700	C	-0.35801100	4.37510100	-3.59682900
O	-2.40849500	1.27073700	0.75100800	H	-2.03745100	3.47902300	-2.64224300
O	-3.06960500	-0.72366000	-0.74819400	C	1.40598600	5.23255100	-2.17858200
P	-1.78716500	0.16935400	-0.29168700	C	0.90166400	5.02489300	-3.43603200
O	-1.11266300	0.74495100	-1.47798500	H	-0.73526600	4.17755200	-4.59678200
O	-0.98540400	-0.77040100	0.68488600	H	2.37948400	5.69652600	-2.04108000
H	-0.01803400	-0.49134500	0.84614200	H	1.46200700	5.34107000	-4.31226800
C	-3.96903900	-3.30129900	-2.44266500	H	-4.68410000	-2.67916600	-1.91732500
C	-2.85233500	-3.83328700	-1.72068900	H	-2.61054500	3.49808700	2.39853100
C	-4.15209000	-3.56786600	-3.77446000	C	6.52338000	-2.75560000	1.85588500
C	-2.63218400	-3.57614900	-0.34400100	C	6.87064100	-2.27758700	0.58843500
C	-1.94024200	-4.69212700	-2.44203700	C	6.00109900	-1.45093400	-0.13226400
C	-3.23396200	-4.39188300	-4.48589500	C	4.76995800	-1.07715900	0.42575600
H	-5.00822800	-3.14833800	-4.29597800	C	4.41780600	-1.63262300	1.68788100
C	-1.53047200	-4.16962200	0.32188800	C	5.27756300	-2.44660000	2.41524300
C	-0.87151600	-5.28565900	-1.76453800	H	7.21621600	-3.38425500	2.40829800
C	-2.16297400	-4.93947000	-3.83317600	H	7.82706600	-2.55233900	0.15182500
H	-3.39283800	-4.58787400	-5.54282200	H	6.27278600	-1.12871900	-1.13069100
C	-1.23384300	-3.92755500	1.70362900	H	4.99631600	-2.83206900	3.39020300
C	-0.64931100	-5.05701300	-0.40398400	C	2.58645900	-0.48168700	0.96187400
H	-0.20093200	-5.94779500	-2.30864000	C	3.62843900	-0.30868400	-0.04351800
H	-1.45949000	-5.57981600	-4.36009600	N	3.10697600	-1.25795900	1.98750400
C	-0.18318400	-4.54834500	2.32886000	C	2.35352700	-1.62471200	3.17916500
H	-1.85155900	-3.22881200	2.25444800	H	1.29776000	-1.56985600	2.89888300
C	0.43304100	-5.68893900	0.28785800	H	2.57718000	-2.66989800	3.41945300
C	0.65890300	-5.45130000	1.61754700	C	2.62528000	-0.73611100	4.38123900
H	0.01285400	-4.34879400	3.37906600	C	2.31433800	0.63061100	4.32825000
H	1.07035300	-6.37108700	-0.27020900	C	3.16647300	-1.26374800	5.55762200
H	1.47948700	-5.94396200	2.13231900	C	2.55038100	1.44916800	5.43149900
C	-1.59773600	3.87585000	2.47461100	H	1.88232200	1.04459200	3.42115400
C	-0.86523000	4.14153100	1.27283500	C	3.40118600	-0.44455900	6.66533700
C	-1.04741600	4.09359600	3.71058600	H	3.40476900	-2.32439300	5.61172100
C	-1.40266500	3.92488000	-0.02048900	C	3.09518600	0.91488700	6.60318200
C	0.46814200	4.68397400	1.41104800	H	2.30185100	2.50570500	5.37521100
C	0.27721200	4.60146500	3.83986700	H	3.82454700	-0.86904700	7.57204400
H	-1.62702800	3.87991300	4.60456400	H	3.27805400	1.55509900	7.46235000
C	-0.63577200	4.24507400	-1.16889500	O	1.42950200	0.01123700	1.01220200

C	5.72742700	3.06637300	-3.70118300	H	-2.19778200	0.59073200	-3.19495200
C	6.47218700	2.29857900	-2.78494000	H	-3.77802200	1.22134400	-3.68020300
C	5.84111800	1.42698700	-1.90537500	C	-3.55106200	-0.90674900	-3.96490800
C	4.43964400	1.30039400	-1.93310000	C	-2.89721000	-2.09582100	-3.60966000
C	3.71129800	2.11189200	-2.84850000	C	-4.44451500	-0.92275200	-5.04056900
C	4.34077300	2.98822100	-3.74040100	C	-3.14789400	-3.27544100	-4.30939800
H	6.24340400	3.74072100	-4.37971700	H	-2.18368300	-2.08731800	-2.79019200
H	7.55359600	2.39746600	-2.75789000	C	-4.69427400	-2.10331100	-5.74570800
H	6.42885900	0.87946600	-1.17964800	H	-4.94666900	-0.00338900	-5.33559900
H	3.75922600	3.59530000	-4.42809700	C	-4.04906700	-3.28387200	-5.37849900
C	2.17914400	0.98433800	-1.62806600	H	-2.63412900	-4.18986500	-4.02387300
C	3.46639800	0.58760800	-1.12075200	H	-5.39275900	-2.09812300	-6.57836500
N	2.36457700	1.91723800	-2.62732200	H	-4.24228500	-4.20430500	-5.92302500
H	1.62759700	2.50697900	-2.98800000	O	-1.57112600	-0.07894100	-0.98108900
H	1.24740900	0.96596700	-1.08732100	C	-3.15316300	2.69028000	5.27007400
C	2.74658000	-2.60622100	-2.03232500	C	-4.28111400	2.74714600	4.42855900
C	1.56974700	-1.94973600	-1.78922600	C	-4.32395000	2.00334700	3.25694100
C	1.49674600	-0.86316800	-2.70134300	C	-3.23761200	1.17441500	2.91430000
C	2.59447200	-1.05827100	-3.62807300	C	-2.09835000	1.14677600	3.77022000
O	3.40126300	-2.07524000	-3.10866100	C	-2.05433200	1.90317500	4.95038600
H	0.86611100	-2.18408900	-1.00430300	H	-3.14045400	3.27520400	6.18650400
H	0.58830300	-0.33230000	-2.94941500	H	-5.12176000	3.38029000	4.69671900
C	2.90910400	-0.46528500	-4.79168400	H	-5.18120200	2.08553300	2.60145500
C	3.39167800	-3.78230800	-1.39906900	H	-1.18070900	1.86558200	5.59446700
H	2.77954500	-4.15067500	-0.57289500	C	-1.56797200	-0.24542100	2.01083800
H	3.52616400	-4.58787200	-2.13228200	C	-2.90059300	0.41855000	1.72590100
H	4.38458400	-3.51562100	-1.01522500	N	-1.11510900	0.32192200	3.27528400
H	3.80422700	-0.73841800	-5.33782400	H	-0.14911700	0.63706800	3.28254600
H	2.26124000	0.29790500	-5.20245000	H	-0.83388500	-0.05092300	1.23543400
22				C	-2.73387700	-2.29059600	3.15883000
C	-7.34735000	0.76566700	-1.28402400	C	-1.68657400	-1.82988900	2.15415000
C	-7.33714000	0.69565300	0.11164000	C	-2.15579500	-2.54129900	0.91624000
C	-6.13388800	0.55457700	0.81185300	C	-3.34191600	-3.10884600	1.16245700
C	-4.92551800	0.51238700	0.10946500	O	-3.76179700	-2.93421100	2.47293400
C	-4.96938100	0.52615400	-1.30653700	H	-0.68455600	-2.14370800	2.46762400
C	-6.15707100	0.66202300	-2.01474100	H	-1.62965200	-2.55444400	-0.02570700
H	-8.28930800	0.87535200	-1.81423500	C	-4.28521700	-3.87601400	0.30449900
H	-8.27311500	0.73733400	0.66149900	H	-3.88632400	-3.97530700	-0.70805200
H	-6.14839800	0.44596100	1.89043500	H	-5.25401900	-3.36453800	0.24956300
H	-6.17005900	0.65960500	-3.09944600	H	-4.46685100	-4.87613100	0.71709600
C	-2.77932800	0.12638000	-0.76212000	C	-2.76343100	-2.19594300	4.48742200
C	-3.53502000	0.29847500	0.50398700	H	-1.96025800	-1.69998300	5.01616600
N	-3.67359400	0.34029200	-1.79986900	H	-3.59693800	-2.59487500	5.05561500
C	-3.27019400	0.37684800	-3.20145300	C	5.41440400	3.06433600	0.07148700

C	4.57533600	2.08487500	-0.48211600	H	3.68112900	-4.26600600	5.49670300
C	3.20949800	2.34025500	-0.57852800	C	1.35913400	-3.84227800	-1.71702700
C	2.67610500	3.60888700	-0.28459200	C	0.81968500	-4.89848900	0.43923800
C	3.56223600	4.59193500	0.18753400	H	0.40599800	-5.71620100	2.38372200
C	4.91419100	4.31964400	0.40375400	H	1.71707600	-5.28893300	4.39322500
C	6.81895300	2.52440600	0.23933400	C	0.29403300	-4.48217600	-2.29730300
C	6.62323000	1.00615100	0.02217500	H	1.96411400	-3.16335300	-2.30576400
C	5.41207200	0.90353800	-0.96453300	C	-0.28053600	-5.54830100	-0.20443500
H	3.16507000	5.57636600	0.41698700	C	-0.53224400	-5.35945600	-1.53673400
H	5.56368000	5.08381400	0.82337500	H	0.07303700	-4.31432600	-3.34823900
H	7.50477400	2.95053900	-0.50630400	H	-0.91417300	-6.19783100	0.39437400
H	6.34752500	0.52830900	0.96929800	H	-1.36526900	-5.86793800	-2.01541300
H	7.51767700	0.50297000	-0.35842800	C	1.44609000	3.70760200	-2.95646200
H	7.24093300	2.75851000	1.22339700	C	0.67932800	3.98068800	-1.77792300
C	5.91259800	1.14591600	-2.43017600	C	0.88283800	3.75602100	-4.20525700
H	6.64918200	1.95290500	-2.49120600	C	1.22780500	3.93218000	-0.47159300
H	5.05490900	1.42819900	-3.05161700	C	-0.70895400	4.34218200	-1.95534200
C	6.45829200	-0.22222300	-2.88863000	C	-0.49219400	4.08760200	-4.37131100
C	5.58634600	-1.19121700	-2.12109200	H	1.49084300	3.54254600	-5.08040400
C	4.89678900	-0.52894000	-1.09189700	C	0.42408400	4.24969400	0.65052200
C	5.40939000	-2.55357500	-2.33801100	C	-1.48294600	4.66941600	-0.83852800
H	5.95315600	-3.06556900	-3.12790900	C	-1.25994300	4.37647600	-3.27511900
C	4.52073100	-3.25918200	-1.52745100	H	-0.92218200	4.12022000	-5.36887400
H	4.38588600	-4.32692000	-1.67278000	C	0.91002500	4.18778000	1.99723400
C	3.75984800	-2.62057800	-0.53388600	C	-0.95353300	4.64210100	0.45408800
C	3.95051500	-1.23676000	-0.35144900	H	-2.52355500	4.95503600	-0.97935700
H	7.51776700	-0.34096000	-2.62120400	H	-2.30757400	4.64714100	-3.38659700
H	6.38980900	-0.36416000	-3.97321500	C	0.11283700	4.53128800	3.05759500
O	2.35186900	1.30203200	-0.95584000	H	1.92107000	3.84116800	2.17200200
O	3.19440900	-0.56979200	0.61364600	C	-1.75099100	4.99081100	1.58911800
P	1.87218100	0.28784400	0.23233200	C	-1.23401400	4.94870600	2.85505900
O	1.32171600	0.93316100	1.44550700	H	0.50681000	4.47315800	4.06889600
O	0.97124900	-0.72638500	-0.58008300	H	-2.78410900	5.28512600	1.42092600
H	0.02444000	-0.43989200	-0.72011000	H	-1.85233200	5.20719100	3.70932100
C	4.18960400	-3.08681400	2.34236300	H	4.89402600	-2.48503900	1.77980900
C	3.05508000	-3.63926800	1.66457900	H	2.49720700	3.46320500	-2.85259200
C	4.40264200	-3.30913400	3.67783300	23-ts			
C	2.80280000	-3.42615500	0.28656100	C	-3.05333700	4.69533800	1.82187500
C	2.15639500	-4.46893700	2.43538800	C	-2.68949700	3.34120400	1.77363100
C	3.49829500	-4.10489000	4.43774800	C	-1.42956400	2.98636700	1.29590600
H	5.27214100	-2.87593900	4.16502300	C	-0.47124100	3.96618000	0.97490800
C	1.68710000	-4.04012500	-0.33575400	C	-0.85248700	5.31438700	1.09177900
C	1.06959400	-5.07934800	1.80241900	C	-2.13822900	5.68687000	1.48333100
C	2.41034800	-4.66962700	3.82897800	C	-4.49770000	4.84171900	2.24825900

C	-5.03854600	3.40555900	2.08072000	H	-3.10625800	-2.91755700	0.81715400
C	-3.80317200	2.47911500	2.35334200	C	-3.72306800	-4.73505100	-2.56873600
H	-0.11955600	6.07743200	0.84671200	C	-3.03492500	-5.36056700	-1.56390500
H	-2.41427000	6.73758900	1.52380400	H	-2.24081000	-5.17539200	0.45478500
H	-4.57278600	5.17804000	3.29221600	H	-3.88705200	-5.23093800	-3.52292400
H	-5.36821900	3.25517600	1.04615800	H	-2.64527900	-6.36492100	-1.70816000
H	-5.88469100	3.17848600	2.73661400	C	1.45821400	2.75638400	2.83695500
H	-5.04412100	5.57328000	1.64204000	C	1.83787400	3.10647100	1.50081900
C	-3.63361000	2.27358300	3.89501100	C	2.36240300	2.22753800	3.72162200
H	-3.78029200	3.20020500	4.45891800	C	0.92919000	3.64821500	0.55827400
H	-2.61509500	1.91946500	4.09175200	C	3.22124100	2.91521400	1.12887600
C	-4.65083600	1.16783900	4.25321100	C	3.71728100	2.01199800	3.33858300
C	-4.72407400	0.35997100	2.97454600	H	2.04491100	1.97298800	4.72972500
C	-4.10030400	1.04594900	1.91969800	C	1.37293400	3.99345500	-0.74126600
C	-5.30137600	-0.88858100	2.76840400	C	3.65271800	3.30170200	-0.14368900
H	-5.79272800	-1.41670800	3.58173400	C	4.13069100	2.35251600	2.07864600
C	-5.26413800	-1.44665100	1.49079100	H	4.41780900	1.58236700	4.04936900
H	-5.75556400	-2.39622700	1.30088300	C	0.49015600	4.48868500	-1.75587500
C	-4.58304000	-0.82533800	0.42993800	C	2.76792100	3.83702500	-1.08373900
C	-3.94809600	0.40566400	0.68962100	H	4.69987300	3.17678800	-0.40890900
H	-5.63043700	1.59256600	4.51380500	H	5.16241800	2.19965000	1.77203600
H	-4.33372800	0.56355500	5.11114600	C	0.95509600	4.84259500	-2.99532500
O	-1.13612300	1.63072500	1.14253800	H	-0.56876500	4.55404200	-1.53872100
O	-3.18175900	0.99701400	-0.31434000	C	3.21646900	4.23346500	-2.38464200
P	-1.55345900	0.93188300	-0.28395400	C	2.33933200	4.72692000	-3.31434800
O	-0.98113400	1.56237500	-1.48827200	H	0.26093600	5.20572600	-3.74831600
O	-1.23991300	-0.58959300	0.03647400	H	4.27513400	4.13397200	-2.61256100
H	-0.25425100	-0.78775700	0.03740000	H	2.69254200	5.03131500	-4.29664700
C	-5.95446600	0.46253900	-1.83470700	H	-5.89869500	0.97024000	-0.87918100
C	-5.32832700	-0.81762100	-1.97830700	H	0.43357900	2.92012700	3.15077900
C	-6.62509100	1.05335300	-2.87380700	C	5.63263000	-3.05637400	3.34513500
C	-4.62270300	-1.45667900	-0.92589000	C	6.48338600	-2.76713500	2.27530100
C	-5.46408500	-1.48291000	-3.25468100	C	5.99768000	-2.13879900	1.12372200
C	-6.72813700	0.40559400	-4.13739500	C	4.64966900	-1.77017000	1.04358600
H	-7.08650800	2.02718000	-2.73324000	C	3.79750800	-2.13278200	2.12047300
C	-4.06394200	-2.74327900	-1.12616800	C	4.26746300	-2.75618800	3.27005500
C	-4.93120100	-2.76407000	-3.42393100	H	6.02381400	-3.54264800	4.23443300
C	-6.16656500	-0.82965000	-4.31574000	H	7.53266900	-3.04375500	2.32873800
H	-7.25973600	0.89147700	-4.95112600	H	6.66556300	-1.97975200	0.28611300
C	-3.30584200	-3.42516800	-0.11899100	H	3.59440900	-3.03022800	4.07518300
C	-4.24718600	-3.41483500	-2.39416100	C	2.42650300	-1.26892400	0.51354300
H	-5.05946500	-3.26996000	-4.37898100	C	3.81145000	-1.16379200	0.01073800
H	-6.24802500	-1.34433500	-5.27036700	N	2.47953100	-1.80436800	1.79038800
C	-2.81459500	-4.68783900	-0.32753000	C	1.30636800	-2.04092700	2.62006300

H	1.49352000	-1.62248300	3.61572300	C	-1.14718600	-3.59282700	1.43689400
H	0.49599500	-1.45965900	2.17141100	C	0.17369700	-3.29774900	1.77603100
C	0.92005900	-3.50711200	2.73374500	C	0.82146200	-2.18921100	1.20900800
C	0.81401800	-4.11978800	3.98662300	C	0.13394300	-1.38979700	0.30472200
C	0.65731000	-4.26565200	1.58390900	C	-1.19180300	-1.70964800	-0.03353300
C	0.46484100	-5.46819600	4.09738900	C	-1.85320700	-2.79997700	0.52282100
H	1.00712600	-3.53755400	4.88560600	H	-1.64191700	-4.44975100	1.88618400
C	0.32129900	-5.61562300	1.69221800	H	0.70535800	-3.92797400	2.48320400
H	0.70864000	-3.79752700	0.60426000	H	1.84879100	-1.96051300	1.47460800
C	0.22440000	-6.22159800	2.94861700	H	-2.88407200	-3.02478200	0.27094000
H	0.38906600	-5.92832600	5.07909300	C	-0.70331900	0.13210300	-1.32372200
H	0.13343300	-6.19578000	0.79246800	C	0.55934200	-0.14761500	-0.46095000
H	-0.03744400	-7.27321100	3.02915600	N	-1.67252300	-0.79685000	-0.98678600
O	1.36939300	-0.92838200	-0.05315300	C	-2.97786100	-0.84055200	-1.63314900
C	7.27536100	1.81100900	-2.92033100	H	-3.16273600	-1.86161800	-1.98791200
C	7.60856100	1.11507700	-1.74531100	H	-2.88516700	-0.19090300	-2.50947100
C	6.66196300	0.34448700	-1.07584300	C	-4.12181600	-0.37765100	-0.74735800
C	5.35013800	0.25054900	-1.57551700	C	-5.23920300	-1.19241700	-0.53877600
C	5.03143200	1.00684600	-2.74014400	C	-4.08497400	0.89046800	-0.15066500
C	5.98164000	1.76742700	-3.42985700	C	-6.30315500	-0.75478500	0.25445700
H	8.03253600	2.39958700	-3.43122900	H	-5.28130900	-2.17564200	-1.00358800
H	8.61804000	1.18208600	-1.34996900	C	-5.14369500	1.32756200	0.64398200
H	6.93860500	-0.14572700	-0.15271400	H	-3.22549500	1.53509500	-0.31597800
H	5.70956100	2.31664700	-4.32706500	C	-6.25599600	0.50580200	0.84961800
C	3.10910200	0.00360200	-2.08265300	H	-7.16402400	-1.40016200	0.40811800
C	4.10784100	-0.36446100	-1.10902000	H	-5.10343900	2.31315600	1.10022100
N	3.68791000	0.86688500	-3.00542800	H	-7.08064300	0.84856600	1.46885800
H	3.15308600	1.50727700	-3.57325600	O	-0.83518400	0.99539000	-2.17654500
H	2.05787600	0.09479400	-1.85993600	C	1.84864200	5.13315900	0.06888200
C	0.60846900	-2.30299300	-3.28243300	C	1.61387800	4.44810800	-1.14058100
C	1.57327900	-1.59918900	-3.93166600	C	1.26766800	3.10267400	-1.15590000
C	2.81549800	-1.82192300	-3.23145300	C	1.15884700	2.40567200	0.06448400
C	2.51314300	-2.84156300	-2.26381700	C	1.38803500	3.12662400	1.27088400
O	1.14094000	-3.05367900	-2.26447200	C	1.73270900	4.48254700	1.29081900
H	1.40888900	-0.93157100	-4.76606300	H	2.11550600	6.18631500	0.04659900
H	3.79750800	-1.72499500	-3.67580900	H	1.69496300	4.98743300	-2.08042300
C	3.30560600	-3.47136100	-1.36281500	H	1.03961200	2.60528100	-2.09101000
H	2.89773000	-4.19018600	-0.66160300	H	1.90154700	5.00643900	2.22837500
H	4.38022400	-3.37537700	-1.42264900	C	0.87058100	1.00662200	1.81856000
C	-0.86475100	-2.38078000	-3.44038900	C	0.83935600	1.04063500	0.44396600
H	-1.36184400	-1.96624300	-2.55537200	N	1.19905000	2.24798200	2.31776100
H	-1.18573400	-1.81079300	-4.31563100	H	0.68319400	0.18006900	2.48711900
H	-1.19960800	-3.41904300	-3.54305800	H	1.28446100	2.47558100	3.29569800
3-S				C	1.74048500	-0.42309900	-1.46250000

H	1.43483500	-1.22316400	-2.14554300	O	-1.43675800	-1.63000200	-1.46184600
H	1.87331300	0.48003300	-2.06449400	P	-1.42053700	-0.41922600	-0.39828900
C	3.03358800	-0.81528300	-0.83183600	O	-1.25584800	0.88120000	-1.10349400
C	4.00951900	-0.14090600	-0.15687400	O	-0.29269400	-0.79931200	0.65739000
O	3.36678900	-2.14804600	-0.90054900	H	0.13566500	-0.02125100	1.09798700
C	4.99842500	-1.11109800	0.21372800	C	-0.11366500	-3.09354400	-3.99293100
H	4.02002800	0.92026200	0.04827900	C	1.04505000	-2.85094500	-3.18615800
C	4.56578900	-2.31502900	-0.26156500	C	-0.10451400	-2.87168300	-5.34567200
H	5.91791000	-0.93349700	0.75521800	C	1.07239900	-3.06633300	-1.78351200
C	5.12414600	-3.69576200	-0.23431300	C	2.24085500	-2.39803000	-3.86101800
H	6.07073200	-3.70291600	0.31361400	C	1.06814000	-2.39649800	-5.99896400
H	5.31328700	-4.07549400	-1.24651700	H	-0.99873600	-3.06866800	-5.93049200
H	4.43935300	-4.39991500	0.25501800	C	2.26768100	-2.84811400	-1.05370700
24-ts				C	3.41755000	-2.21482500	-3.12903600
C	-5.73083000	-1.74171200	-1.31329100	C	2.20715700	-2.17302200	-5.27352100
C	-4.50286700	-1.76545000	-0.63157300	H	1.05687100	-2.23018200	-7.07255600
C	-4.02876400	-0.58831900	-0.05397900	C	2.35532400	-3.01577900	0.36715900
C	-4.82273600	0.57362100	0.00550300	C	3.46598000	-2.43730400	-1.75072300
C	-6.08047600	0.52929200	-0.62438200	H	4.32017700	-1.89893900	-3.64698300
C	-6.52277700	-0.59866200	-1.31197100	H	3.11777300	-1.83239800	-5.76060200
C	-5.99994400	-3.07181000	-1.98033000	C	3.53832800	-2.83831500	1.03781900
C	-4.62856200	-3.77284100	-1.89137300	H	1.46107200	-3.28526900	0.91631400
C	-3.97389300	-3.19635400	-0.58877700	C	4.68226300	-2.27259400	-1.01518700
H	-6.70929600	1.41283900	-0.57756900	C	4.72464200	-2.47308600	0.33820000
H	-7.48111300	-0.58475500	-1.82419800	H	3.57096700	-2.97744900	2.11435500
H	-6.77548300	-3.63512100	-1.44353700	H	5.57761200	-1.98996900	-1.56335000
H	-4.01091500	-3.49022800	-2.75189000	H	5.65573700	-2.35094200	0.88443800
H	-4.69755900	-4.86432200	-1.87574200	C	-4.38290100	0.60134700	2.92923000
H	-6.35199700	-2.95886100	-3.01171400	C	-4.28638500	1.79926900	2.14961000
C	-4.52532000	-3.96995200	0.65632400	C	-4.22289300	0.61820800	4.29043300
H	-5.60307000	-4.14656900	0.59440400	C	-4.44379700	1.82080700	0.73921800
H	-4.33599900	-3.37378900	1.55657700	C	-4.05762900	3.03763000	2.86167300
C	-3.69227500	-5.27028800	0.70482500	C	-3.96182900	1.83629100	4.98020900
C	-2.37524100	-4.84186200	0.09424400	H	-4.30490800	-0.30704100	4.85400600
C	-2.50128600	-3.58210700	-0.51473800	C	-4.38614900	3.05321500	0.03767000
C	-1.15897000	-5.51711100	0.08135600	C	-4.04283900	4.24568500	2.15787600
H	-1.06328200	-6.49865300	0.53815400	C	-3.88840900	3.01095700	4.28209000
C	-0.06251500	-4.92962400	-0.55077000	H	-3.83937600	1.82882000	6.05959400
H	0.87906100	-5.46687900	-0.61109100	C	-4.48449500	3.14255000	-1.39057700
C	-0.12861000	-3.63676500	-1.09893300	C	-4.21594600	4.28810600	0.77138700
C	-1.36117900	-2.96370700	-1.01766400	H	-3.91215600	5.17680400	2.70577000
H	-4.16148400	-6.07081600	0.11690300	H	-3.71340100	3.95277800	4.79654300
H	-3.57442100	-5.65801900	1.72284900	C	-4.47351500	4.35314300	-2.03537800
O	-2.74526300	-0.58407200	0.51934100	H	-4.56179200	2.22814900	-1.96707100

C	-4.22323100	5.53156300	0.06204500	H	2.56581500	1.82916600	-4.90465100
C	-4.35815500	5.56917500	-1.30102800	C	1.71879600	2.03673300	-0.86939700
H	-4.55455500	4.38829400	-3.11835100	C	3.11640600	1.61920800	-0.46405200
H	-4.12380300	6.45052200	0.63515300	N	1.67041300	2.00585800	-2.25326300
H	-4.37434900	6.52022300	-1.82622600	H	0.80956800	1.74126800	-2.71803400
H	-1.01302500	-3.47235700	-3.52180100	H	0.86439200	1.61465700	-0.36253300
H	-4.59819600	-0.33576100	2.43041500	C	0.37106400	4.26163400	-0.73613800
C	6.68162100	0.63010400	3.47144500	C	1.62869700	3.79896700	-0.21991900
C	7.02825200	1.11602800	2.20830100	C	2.62297800	4.59787700	-0.95254700
C	6.04380700	1.38071000	1.25277700	C	1.97597000	5.25605900	-1.92742100
C	4.69789900	1.14214100	1.55567900	O	0.57877700	5.02489400	-1.78623900
C	4.37388000	0.71711600	2.86876000	H	1.69689400	3.58018000	0.83965400
C	5.33962100	0.43916800	3.82444800	H	3.69156200	4.58413200	-0.79677100
H	7.45763100	0.41654400	4.20025800	C	2.35619200	6.14777700	-3.04990300
H	8.07052200	1.29805100	1.96610500	H	2.07318600	5.71168500	-4.01505600
H	6.33420200	1.81228200	0.30440300	H	1.86117100	7.12206100	-2.96608200
H	5.07050700	0.08533600	4.81268900	H	3.43754900	6.30433300	-3.04537000
C	2.36518100	1.11910000	1.87807400	C	-1.00624700	3.93594000	-0.34895900
C	3.43908300	1.35684900	0.84787400	H	-1.27624100	2.93055600	-0.71627700
N	2.97659800	0.69607600	3.02488000	H	-1.09624600	3.89615900	0.74126700
C	2.25319400	0.46006700	4.28160900	H	-1.71169600	4.66018600	-0.76004500
H	2.74597800	1.04867100	5.06334100	25			
H	1.25669400	0.88021500	4.12250200	C	5.57309600	-1.81576900	1.69154700
C	2.15984500	-0.99578300	4.69888300	C	4.68357200	-1.59509400	0.62692800
C	2.80236200	-1.44439000	5.85788500	C	4.10949700	-0.33411200	0.47749700
C	1.39186100	-1.90114000	3.95284100	C	4.48434800	0.74874500	1.29438400
C	2.69650400	-2.77780600	6.26132200	C	5.42939900	0.50086100	2.30524400
H	3.37859400	-0.74535100	6.46089700	C	5.95323700	-0.77196600	2.52833400
C	1.28591000	-3.23296900	4.35361600	C	5.97674000	-3.27207200	1.75586400
H	0.86816700	-1.56520000	3.06192300	C	4.93330800	-3.94549700	0.84006900
C	1.94113600	-3.67544100	5.50675300	C	4.58357500	-2.85367200	-0.22927000
H	3.20003700	-3.11077200	7.16440900	H	5.73451600	1.32946500	2.93718200
H	0.68295700	-3.92373500	3.77055100	H	6.65039800	-0.93950700	3.34507800
H	1.85527400	-4.71243000	5.81863200	H	6.99725800	-3.41860700	1.37624300
O	1.13177000	1.25345000	1.75907600	H	4.03033000	-4.17833700	1.41686900
C	4.62979800	1.38314100	-4.41593000	H	5.28654400	-4.87622100	0.38664100
C	5.56383800	1.15525000	-3.39498800	H	5.96282700	-3.66772600	2.77746300
C	5.18809000	1.22804500	-2.05538400	C	5.66441700	-2.87070500	-1.36163900
C	3.86254900	1.54990300	-1.72002000	H	6.67944100	-2.97755300	-0.96806400
C	2.93684300	1.75111700	-2.77694100	H	5.61655200	-1.92377300	-1.91142600
C	3.29848500	1.67645400	-4.11834400	C	5.23783200	-4.03345700	-2.28485000
H	4.94274400	1.32349200	-5.45426800	C	3.73300700	-4.04370400	-2.12446400
H	6.59053200	0.91142800	-3.64921400	C	3.34798200	-3.25140700	-1.03002700
H	5.91495700	0.99601000	-1.29144400	C	2.77979000	-4.69423300	-2.90118600

H	3.07724000	-5.32285400	-3.73617400	C	4.40557300	5.10039800	-1.16711900
C	1.42889900	-4.53167000	-2.59505600	H	5.54580700	5.18432900	-2.97168000
H	0.67650100	-5.05225200	-3.17972900	C	2.71200800	1.97720800	3.29600700
C	1.00202100	-3.67448100	-1.56577000	C	2.75810600	4.09889200	2.04998100
C	1.99261000	-3.01999300	-0.80840300	H	2.87447800	5.90122800	0.88455600
H	5.67963600	-4.98616800	-1.96260800	H	4.10245200	6.14403200	-1.20494300
H	5.54485800	-3.88169200	-3.32545400	C	1.97101000	2.57215000	4.28469300
O	3.12357300	-0.14914800	-0.51201400	H	2.98038200	0.93068700	3.37777400
O	1.60062400	-2.11738400	0.19115600	C	1.97684500	4.67988300	3.09832900
P	1.60490500	-0.51401800	-0.10306700	C	1.60233000	3.94579500	4.19175100
O	1.04460300	0.16862800	1.09270000	H	1.67043500	1.99458100	5.15570300
O	0.88642000	-0.27045500	-1.49115800	H	1.70255200	5.72865600	3.01375200
H	-0.06495400	0.01147800	-1.36458100	H	1.03916600	4.41152000	4.99699100
C	-0.29085200	-4.55298100	0.94281400	H	0.77960600	-4.66532400	0.81692100
C	-1.05298200	-3.96525300	-0.11946400	H	5.54589400	1.38462000	-0.96642000
C	-0.88519700	-4.98792000	2.10039600	C	-5.94280800	3.65171300	-2.98397100
C	-0.46435300	-3.50216600	-1.32402400	C	-6.59655100	3.39506500	-1.77632300
C	-2.48669400	-3.88263700	0.05575500	C	-6.03351600	2.53243800	-0.83127600
C	-2.29671000	-4.88466300	2.27668800	C	-4.81195400	1.90627200	-1.10349100
H	-0.28086600	-5.43894700	2.88248700	C	-4.13273400	2.24970100	-2.29738100
C	-1.28298500	-2.95384000	-2.34517800	C	-4.68752500	3.09298200	-3.25192400
C	-3.27990700	-3.36549000	-0.97349000	H	-6.39681000	4.31269000	-3.71601600
C	-3.07192700	-4.35475600	1.27633900	H	-7.54772700	3.87310700	-1.56380100
H	-2.75461300	-5.26149700	3.18749700	H	-6.53597700	2.38426000	0.11687400
C	-0.75058700	-2.42994300	-3.56906900	H	-4.16319100	3.33386500	-4.17062500
C	-2.71734100	-2.90388800	-2.16704200	C	-2.66054100	0.95706300	-1.13579800
H	-4.36000500	-3.33052500	-0.84694200	C	-3.92927400	1.01063700	-0.35123600
H	-4.15463700	-4.31154800	1.37708100	N	-2.85992900	1.65058300	-2.29940900
C	-1.57191200	-1.94054700	-4.55281500	C	-1.85300900	1.76746200	-3.35968400
H	0.32308000	-2.41887400	-3.71083500	H	-1.33371300	0.80761100	-3.41361800
C	-3.53843500	-2.38591300	-3.21803800	H	-2.40330900	1.87959700	-4.29992900
C	-2.98676300	-1.92600900	-4.38338900	C	-0.85309000	2.89687500	-3.17271000
H	-1.14016400	-1.56050600	-5.47473900	C	0.51730300	2.61628600	-3.21507400
H	-4.61561000	-2.37387300	-3.07142100	C	-1.26888400	4.22534100	-3.00055100
H	-3.62128400	-1.54763200	-5.17991300	C	1.45810100	3.64079500	-3.09130900
C	5.21029300	2.41414000	-1.01801500	H	0.85575500	1.59107000	-3.33473600
C	4.36662400	2.92201500	0.02216400	C	-0.33018100	5.24900300	-2.87571800
C	5.61226400	3.20593100	-2.06275500	H	-2.32726100	4.46613100	-2.95977900
C	3.95758400	2.14039100	1.13080300	C	1.03554500	4.95917500	-2.92344000
C	3.96072700	4.30690900	-0.06278400	H	2.51803100	3.40677700	-3.11465400
C	5.20653100	4.56955400	-2.14276500	H	-0.66652200	6.27420500	-2.74589500
H	6.25748100	2.79525400	-2.83446000	H	1.76791500	5.75527000	-2.82668500
C	3.15404600	2.71213900	2.14774000	O	-1.61746100	0.34334100	-0.83965300
C	3.16691400	4.85527600	0.94830900	C	-7.32668600	-1.60947700	2.84709000

C	-7.69098700	-0.78605000	1.76801700	H	2.49510100	-6.93964200	0.45012500
C	-6.72284400	-0.11623000	1.03019100	C	6.21707300	-5.26643500	-0.54359200
C	-5.36312000	-0.25588700	1.37260800	H	6.23289400	-6.24449800	-0.05312100
C	-5.02068900	-1.12111100	2.43994500	H	6.86466300	-4.59382500	0.03061600
C	-5.98961700	-1.79301100	3.18861400	C	6.68258300	-5.30635100	-2.01330900
H	-8.09777200	-2.12059100	3.41627900	C	5.97770900	-4.10554800	-2.60355000
H	-8.73777100	-0.67966700	1.50174700	C	4.95932200	-3.65531000	-1.74856300
H	-7.01934100	0.47257500	0.17345000	C	6.24477200	-3.44926200	-3.79983700
H	-5.70308100	-2.44279000	4.01013300	H	7.01955700	-3.80905600	-4.47216000
C	-2.98873000	-0.47994800	1.50554300	C	5.51378400	-2.30735600	-4.11918600
C	-4.13545700	0.19297900	0.73408700	H	5.71278300	-1.78275800	-5.04877000
N	-3.63795900	-1.22643800	2.59877700	C	4.54432700	-1.77316000	-3.25072400
H	-3.30718900	-2.18456900	2.69508400	C	4.28023000	-2.47455900	-2.05553000
H	-2.42020500	-1.14806000	0.85186200	H	6.37012400	-6.23748400	-2.50695700
C	-1.21073000	-0.00258000	3.25928600	H	7.77205500	-5.24583100	-2.11577200
C	-1.97800200	0.55462900	2.11312800	O	4.86227500	-1.93109500	0.88311500
C	-2.54971300	1.79932000	2.72604300	O	3.30964500	-2.00576600	-1.17270700
C	-2.12308300	1.91575200	3.98145200	P	3.69497500	-1.08212300	0.12030700
O	-1.28737400	0.77243600	4.28615300	O	2.46739500	-0.78819000	0.88936900
H	-1.23696500	0.78426000	1.32332800	O	4.57563300	0.12284700	-0.40250700
H	-3.18742800	2.50161200	2.20942700	H	3.97926800	0.90512200	-0.62292400
C	-2.26387300	2.88079700	5.09581300	C	1.63077200	-1.55038800	-3.80386100
H	-2.94612800	3.68134600	4.80001400	C	2.50635900	-0.42559100	-3.94052400
H	-2.66214700	2.39425200	5.99332800	C	0.29213200	-1.45475300	-4.08541800
H	-1.29486800	3.32532400	5.34925600	C	3.89002700	-0.48376200	-3.64061800
C	-0.36504300	-1.19505600	3.33541400	C	1.93198900	0.80841100	-4.43076600
H	0.51949200	-0.95933200	2.71523000	C	-0.27119900	-0.22783700	-4.54020600
H	-0.07562600	-1.41475200	4.36426900	H	-0.34852900	-2.32307200	-3.96747100
H	-0.83398500	-2.06300600	2.86134700	C	4.70127400	0.66959900	-3.81225200
26-ts				C	2.75446500	1.91911400	-4.63581900
C	3.69947600	-5.39003500	1.40181300	C	0.53083300	0.86769500	-4.71547100
C	4.29905200	-4.27331900	0.79695600	H	-1.33536400	-0.17058800	-4.75075000
C	4.43277700	-3.09420600	1.52939100	C	6.09304800	0.70483600	-3.46687300
C	4.12108600	-3.04811100	2.90181300	C	4.12027200	1.88216000	-4.34366900
C	3.60301200	-4.21261000	3.49345000	H	2.31969400	2.83537600	-5.02975100
C	3.35601000	-5.36793400	2.75042400	H	0.11751000	1.80854500	-5.07032600
C	3.49637000	-6.49808400	0.38944400	C	6.85809500	1.82230100	-3.68425700
C	3.74872800	-5.77394800	-0.95241300	H	6.54118500	-0.16922500	-3.01065200
C	4.77728400	-4.64854400	-0.60270800	C	4.95416700	3.02469700	-4.56134700
H	3.36509000	-4.18950200	4.55287400	C	6.28850600	2.99685800	-4.25479900
H	2.90458400	-6.23621400	3.22380400	H	7.90995300	1.81552400	-3.41076400
H	4.21159500	-7.31824400	0.54232000	H	4.49856100	3.92008100	-4.97776200
H	2.82158400	-5.30527300	-1.30296900	H	6.91277000	3.86847000	-4.43378200
H	4.10560400	-6.43934100	-1.74465200	C	6.82570500	-2.07757900	3.52666500

C	5.66584300	-1.42467600	4.05524100	C	6.81346600	5.19383600	2.36283600
C	8.09094500	-1.65670700	3.84404900	H	6.95613200	5.50960900	0.23670400
C	4.34380100	-1.83563800	3.75068900	C	6.19618600	4.47401800	3.38587000
C	5.87829700	-0.31851800	4.96123500	H	4.76293200	2.92864000	3.86085400
C	8.29294100	-0.55264100	4.72020000	H	7.56730000	5.94096100	2.59718900
H	8.95175200	-2.17092400	3.42495800	H	6.46834400	4.65732900	4.42206100
C	3.23791200	-1.16652600	4.33014800	O	2.79263200	1.97230300	-0.86578100
C	4.77615400	0.31343700	5.54549100	C	-3.20054600	4.05110300	-4.03042900
C	7.21461600	0.09153300	5.26383300	C	-2.10224900	4.90901000	-4.28585400
H	9.30323300	-0.23080100	4.95789100	C	-0.92824000	4.77834100	-3.56333500
C	1.87880400	-1.51235000	4.03397300	C	-0.83302600	3.78713700	-2.56058400
C	3.46642200	-0.08374400	5.26110700	C	-1.93696700	2.90824300	-2.35250900
H	4.94348000	1.12536400	6.25111800	C	-3.13829600	3.04669600	-3.08057600
H	7.35352900	0.92993100	5.94247800	H	-4.11062400	4.17185600	-4.61309600
C	0.83150000	-0.87707000	4.64911000	H	-2.17760900	5.65990000	-5.06648800
H	1.68368800	-2.27294500	3.28829600	H	-0.07738700	5.40777000	-3.79393500
C	2.34516300	0.55199600	5.88282300	H	-3.95768400	2.36062700	-2.89657700
C	1.06466700	0.16040400	5.59789200	C	-0.21108800	1.99949200	-1.11387900
H	-0.18929600	-1.15578000	4.40349900	C	0.25752300	3.33099600	-1.74025600
H	2.53744500	1.35168900	6.59469200	N	-1.62928500	1.95998600	-1.44555000
H	0.22120100	0.63901600	6.08918800	H	-2.28740000	1.20530400	-1.23161500
H	2.04071400	-2.49474900	-3.46560700	H	0.31337400	1.17388500	-1.62008600
H	6.69378200	-2.92564800	2.86463700	C	-0.56558300	0.70546500	1.13787900
C	3.33074400	7.75337400	-1.62423100	C	0.07501600	1.85747000	0.40149100
C	1.95440500	7.74063700	-1.86708200	C	-0.23216100	3.00849700	1.32087700
C	1.23988100	6.53886900	-1.88131300	C	-0.77789500	2.52959300	2.43618300
C	1.91097400	5.32849900	-1.67047700	O	-0.95698200	1.12381600	2.33742700
C	3.29634500	5.37653400	-1.37415400	H	1.15413000	1.62456500	0.45695800
C	4.01779800	6.56422300	-1.35689600	H	0.01878600	4.04079000	1.12699600
H	3.87279800	8.69482900	-1.61984100	C	-1.21621800	3.10846800	3.72948300
H	1.42795200	8.67486400	-2.04107100	H	-1.06032300	4.19001800	3.72228200
H	0.16809800	6.55753800	-2.03861200	H	-2.27902800	2.90835200	3.90660500
H	5.07488300	6.57709000	-1.11537800	H	-0.64365400	2.67437400	4.55801200
C	2.69019700	3.19649400	-1.10267000	C	-0.79453600	-0.61588200	0.76188600
C	1.48665800	3.93424000	-1.51657000	H	-0.30188200	-0.93666100	-0.15240700
N	3.74578000	4.08366600	-1.07570900	H	-0.72513700	-1.34071400	1.57620600
C	5.12303900	3.72502700	-0.73842400	H	-2.12681600	-0.76386500	0.66746800
H	5.24259500	2.66576100	-0.97456100	C	-8.51695600	0.55796000	-1.41887300
H	5.78410500	4.27318200	-1.41612400	C	-7.63612300	-0.18917200	-0.62293500
C	5.49522100	3.99682200	0.70924200	C	-6.74293900	0.47288200	0.21892000
C	4.88674700	3.27200600	1.74393300	C	-6.88722200	1.85161200	0.47526800
C	6.46359500	4.95324600	1.03181800	C	-7.84207300	2.55909200	-0.27636800
C	5.23384100	3.50969400	3.07289300	C	-8.61441500	1.93707500	-1.25933100
H	4.15057200	2.50974300	1.50523900	C	-9.26001100	-0.35070700	-2.37810900

C	-8.51125000	-1.69787900	-2.22673100	C	-0.20865300	-4.57620800	1.27737200
C	-7.96167800	-1.67246400	-0.76454400	C	-0.65229300	-4.40431700	2.56190300
H	-7.95869800	3.62296100	-0.09117600	H	-2.37358800	-4.00339800	3.83298600
H	-9.30065800	2.52276200	-1.86609200	H	0.84503200	-4.75037000	1.07687200
H	-10.31890400	-0.44713000	-2.10030500	H	0.04770500	-4.45429600	3.39170900
H	-7.66533800	-1.73641400	-2.92233300	C	-7.27915300	1.13249500	3.29650600
H	-9.14613000	-2.56865200	-2.42091500	C	-6.39838200	2.19777800	2.92060500
H	-9.24046300	0.02672400	-3.40724800	C	-7.50200500	0.81378900	4.61089100
C	-9.11489900	-2.04718100	0.23454200	C	-6.14495900	2.55449300	1.56912900
H	-10.07960100	-1.62555000	-0.06388800	C	-5.77959400	2.95141400	3.98826500
H	-8.86637500	-1.64232100	1.22251100	C	-6.86571900	1.54217100	5.65540000
C	-9.10588600	-3.58702300	0.29478100	H	-8.17472400	-0.00223100	4.86101600
C	-7.64561800	-3.90542700	0.06684800	C	-5.29238900	3.64758600	1.27588800
C	-6.97375000	-2.79362800	-0.46435600	C	-4.96653000	4.04562700	3.67780000
C	-6.96733000	-5.08940800	0.33578300	C	-6.03387200	2.58424300	5.34731600
H	-7.48963300	-5.95056100	0.74501200	H	-7.05148400	1.27362900	6.69191300
C	-5.59905700	-5.15373900	0.07750700	C	-4.96491000	4.03563800	-0.06342800
H	-5.05302000	-6.07263800	0.27149800	C	-4.71405600	4.41806900	2.35490000
C	-4.88538500	-4.04812000	-0.41401800	H	-4.53283000	4.63056300	4.48710600
C	-5.59364500	-2.85606700	-0.66483800	H	-5.55214200	3.16137700	6.13347900
H	-9.73488700	-4.02216000	-0.49513000	C	-4.17574800	5.12766000	-0.31816300
H	-9.48120300	-3.97745300	1.24773200	H	-5.33768300	3.43371100	-0.88321200
O	-5.69482500	-0.23065300	0.80481100	C	-3.89873000	5.55246500	2.04632900
O	-4.93633800	-1.73860900	-1.15713400	C	-3.64423700	5.90693100	0.74886600
P	-4.39380800	-0.54033300	-0.16536800	H	-3.93940100	5.39244800	-1.34414700
O	-4.01582400	0.60344400	-1.04931800	H	-3.48960300	6.13107300	2.87185000
O	-3.36017600	-1.11010500	0.81439400	H	-3.02756500	6.77408200	0.52692000
C	-3.82939400	-4.38685700	-3.12634600	H	-4.88415600	-4.19133900	-2.96893300
C	-2.95656400	-4.40804200	-1.99079300	H	-7.78420500	0.57199600	2.51933900
C	-3.35854200	-4.61241200	-4.39374800	7-an			
C	-3.41885000	-4.20691400	-0.66860300	C	-1.08048300	3.83780200	-0.07049600
C	-1.55589300	-4.67728500	-2.22447900	C	0.31301300	3.80014800	0.05029200
C	-1.97798900	-4.88202300	-4.61899300	C	1.02852700	2.60843600	-0.12034200
H	-4.04330200	-4.59045600	-5.23731400	C	0.35370300	1.40601800	-0.40924400
C	-2.51601100	-4.26809300	0.41906700	C	-1.07494100	1.48508500	-0.56682700
C	-0.67388200	-4.71846800	-1.14078700	C	-1.78602000	2.66469400	-0.39000400
C	-1.10647000	-4.91381200	-3.56247200	H	-1.62130400	4.77065400	0.07603300
H	-1.62246400	-5.06527900	-5.62942500	H	0.85798900	4.71604100	0.27633400
C	-2.92942000	-4.07960000	1.77799500	H	2.11247500	2.62318100	-0.05726600
C	-1.11479000	-4.52176000	0.17130900	H	-2.86920900	2.68136400	-0.49396400
H	0.38088900	-4.91596300	-1.32204700	C	-0.42193200	-0.67755400	-1.04655000
H	-0.05138800	-5.12632100	-3.72115000	C	0.74745600	0.05088800	-0.66556300
C	-2.03282700	-4.15224300	2.81180900	N	-1.52171700	0.22956000	-0.94044300
H	-3.97027900	-3.85753000	1.97952600	C	-2.85235400	-0.14124800	-1.35558900

H	-3.32508800	0.70459900	-1.87216900	H	3.58408400	-1.98867900	-0.60982200
H	-2.71711200	-0.95822600	-2.07517800	H	2.99515800	-1.18463900	-2.07044200
C	-3.75100100	-0.63046400	-0.22885900	C	4.14149700	0.09047900	-0.74323100
C	-4.95994700	0.00108500	0.07742500	C	5.44010500	-0.18583500	-0.30088400
C	-3.36948500	-1.76023200	0.51254900	C	3.77299000	1.41972500	-0.98706800
C	-5.77906100	-0.47740200	1.10509900	C	6.35915700	0.84801700	-0.10662100
H	-5.26297800	0.87893400	-0.49086300	H	5.73983600	-1.21528400	-0.11522600
C	-4.18469900	-2.23840400	1.53718800	C	4.68741600	2.45323600	-0.78727700
H	-2.43063100	-2.24744000	0.25889500	H	2.76822800	1.64713400	-1.33499700
C	-5.39275900	-1.59926800	1.83851100	C	5.98333200	2.16978600	-0.34730700
H	-6.71413200	0.03005100	1.33395900	H	7.36461700	0.61900700	0.23457700
H	-3.87834100	-3.11459500	2.10483300	H	4.39107000	3.48065900	-0.97916100
H	-6.02539700	-1.97333200	2.64079600	H	6.69512400	2.97572900	-0.19431800
O	-0.60223100	-1.86428200	-1.41615600	O	0.63349800	-0.90425800	-2.38411500
C	5.72329900	-0.32979900	1.50578000	C	-3.83810000	3.56286900	1.09806500
C	4.73334400	0.60757400	1.86256700	C	-3.29693000	2.65896600	2.02708100
C	3.49493900	0.62549700	1.22556600	C	-2.47271600	1.60685300	1.63150500
C	3.21949800	-0.29865200	0.20134400	C	-2.17071000	1.43532800	0.26868500
C	4.23206000	-1.25633300	-0.11894800	C	-2.73172500	2.37393600	-0.63809200
C	5.47997300	-1.27482600	0.51278300	C	-3.55596000	3.43155300	-0.25751400
H	6.68416100	-0.32259200	2.01648400	H	-4.47440300	4.37304100	1.43966500
H	4.93771700	1.32395500	2.65551500	H	-3.51738600	2.78624600	3.08257800
H	2.73610600	1.33901200	1.52786600	H	-2.05856900	0.95527200	2.38573600
H	6.23301700	-2.01387200	0.24342800	H	-3.95686400	4.12634600	-0.98983100
C	2.40531000	-1.70289100	-1.36245200	C	-1.51307700	0.94256400	-1.86554000
C	2.05479900	-0.58898400	-0.62362000	C	-1.37052000	0.50164600	-0.53482800
N	3.71827800	-2.08384400	-1.08876700	N	-2.29962500	2.03223500	-1.91657300
H	4.13671300	-2.95143700	-1.38338900	H	-2.52116400	2.54370800	-2.76037300
H	1.78852100	-2.25907500	-2.05126500	H	-1.04837900	0.53390600	-2.74984100
10-ts-an				C	-1.48600400	-2.35595100	-0.42959700
C	1.89340800	-1.00499800	3.31574800	C	-1.83857600	-2.37777000	-1.81222600
C	0.51230200	-0.97561700	3.52763200	C	-3.10404300	-1.83818000	-1.93818600
C	-0.36499600	-0.84420500	2.44624700	C	-3.56311900	-1.58029500	-0.63496300
C	0.14967200	-0.72823700	1.15399700	O	-2.66161500	-1.97120000	0.26162300
C	1.54363300	-0.83328800	0.96026700	H	-1.17386800	-2.68665000	-2.60597000
C	2.43019900	-0.94614100	2.02383400	H	-3.66465800	-1.65302300	-2.84413800
H	2.56600700	-1.09409600	4.16346400	C	-4.84544900	-1.03172300	-0.13099000
H	0.11614800	-1.06348900	4.53410100	H	-5.38111200	-1.79814300	0.44312800
H	-1.43536400	-0.88767900	2.61116600	H	-4.66325800	-0.18523500	0.54119600
H	3.50127200	-0.98232000	1.86221500	H	-5.47933000	-0.70761300	-0.95859400
C	0.69747300	-0.80003800	-1.16676600	C	-0.71131100	-3.45681200	0.24515300
C	-0.48464800	-0.59819400	-0.18440400	H	-1.27438100	-4.39479300	0.18932100
N	1.84384400	-0.84498800	-0.41512000	H	0.24334300	-3.60509700	-0.26798300
C	3.17285000	-1.04956500	-0.99918100	H	-0.51765100	-3.23002700	1.29409900

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C	1.15281700	-2.58970300	3.13528600
C	-0.23551300	-2.45799500	3.11079600
C	-0.87328800	-1.88734900	2.00153400
C	-0.11211100	-1.45029600	0.92290500
C	1.28257300	-1.63755000	0.94709300
C	1.93318200	-2.18659100	2.04538800
H	1.63966600	-3.02304100	4.00359200
H	-0.82825700	-2.79783300	3.95397000
H	-1.95410600	-1.81851800	1.98669400
H	3.00978500	-2.31375300	2.06377300
C	0.88504300	-0.83075600	-1.15555100
C	-0.47761700	-0.76337000	-0.38953600
N	1.84564700	-1.24827100	-0.28678000
C	3.26777900	-1.32498800	-0.66965500
H	3.71396800	-2.14444700	-0.10046600
H	3.28343000	-1.60218500	-1.72664700
C	4.01888400	-0.02616100	-0.45044000
C	4.69651100	0.22140500	0.74942400
C	4.03943500	0.94754800	-1.45908000
C	5.37625800	1.42476600	0.94449600
H	4.70470500	-0.53157700	1.53392900
C	4.71960900	2.15044900	-1.26515200
H	3.52748600	0.75390900	-2.39801400
C	5.38746000	2.39198000	-0.06226400
H	5.90343500	1.60227400	1.87746800
H	4.74012400	2.89330100	-2.05787600
H	5.92363100	3.32502700	0.08578800
O	1.05052200	-0.54340300	-2.33720500
C	-3.49735200	3.24073900	1.91491100
C	-3.62866200	1.86188600	2.17634800
C	-2.81971600	0.92278600	1.54512500
C	-1.84463500	1.34716200	0.61767600
C	-1.74197800	2.74829200	0.37880400
C	-2.54995600	3.69935100	1.01152400
H	-4.13933700	3.94932200	2.42884900
H	-4.36623800	1.52656700	2.89994500
H	-2.94492400	-0.12449600	1.78557000
H	-2.43645600	4.75912000	0.80138800
C	-0.21614900	1.73135000	-0.91618500
C	-0.84873000	0.70797700	-0.23324800
N	-0.74604300	2.93823500	-0.55507800
H	-0.41591300	3.83414500	-0.88285700
H	0.58475900	1.68057000	-1.63735200

C	-1.52419000	-1.58264600	-1.27740600
C	-1.76535300	-0.95559600	-2.60426800
C	-3.02662900	-0.45542500	-2.65464600
C	-3.63659600	-0.75368600	-1.40080400
O	-2.84037700	-1.42709800	-0.62007400
H	-0.99395200	-0.90784700	-3.36129700
H	-3.51082100	0.06870100	-3.46747900
C	-4.98019300	-0.40194100	-0.90014200
H	-5.43253200	-1.25079200	-0.37748100
H	-4.86516500	0.40862100	-0.16261600
H	-5.62995100	-0.06273400	-1.70858900
C	-1.22386400	-3.08314100	-1.36518700
H	-2.00787300	-3.59999000	-1.92557200
H	-0.27391700	-3.23008900	-1.88609100
H	-1.15204600	-3.51099200	-0.36386900

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C	-6.30837800	-0.25108100	-2.63400000
C	-5.69470900	-0.50474400	-1.39860800
C	-5.03043400	0.52481800	-0.72786600
C	-5.07815200	1.84485600	-1.22706500
C	-5.76318700	2.07594200	-2.43274000
C	-6.35399700	1.03870200	-3.15403000
C	-6.83638100	-1.53414200	-3.23899000
C	-6.13549000	-2.61447100	-2.38685000
C	-5.94280700	-1.95032300	-0.98128700
H	-5.80697400	3.09181300	-2.81557200
H	-6.83985600	1.24078400	-4.10556500
H	-7.93007900	-1.59905900	-3.14681800
H	-5.14741000	-2.83243000	-2.80859200
H	-6.69110000	-3.55630600	-2.33324900
H	-6.60612400	-1.62146500	-4.30739300
C	-7.26088400	-2.09296000	-0.14886900
H	-8.15863700	-1.91453800	-0.74996000
H	-7.24524900	-1.35296500	0.65946300
C	-7.19296500	-3.51638100	0.44762700
C	-5.70240800	-3.73499500	0.60005100
C	-4.98680900	-2.76244000	-0.11389300
C	-5.03653600	-4.70906700	1.33740800
H	-5.58828500	-5.46690700	1.88831700
C	-3.64165300	-4.70188500	1.35761100
H	-3.10508800	-5.47060100	1.90661000
C	-2.89696400	-3.70174600	0.70956100
C	-3.59624500	-2.70270100	0.00134600
H	-7.63891700	-4.25638400	-0.23258300

H	-7.72961500	-3.60192400	1.39977200	H	-3.15626200	2.38311800	-2.84861700
O	-4.34542800	0.24218300	0.43372600	C	-1.83881500	5.65503800	-1.20578300
O	-2.90967500	-1.65171200	-0.57666900	C	-1.34963400	5.24829900	-2.41957400
P	-2.75680400	-0.26529500	0.34115800	H	-1.43195600	3.71874400	-3.96854800
O	-1.99908700	0.67073500	-0.59841500	H	-1.46591300	6.56050800	-0.73190200
O	-2.30366100	-0.52855500	1.73016100	H	-0.58717800	5.83376700	-2.92807100
C	-1.27751300	-4.30337600	-1.67125300	H	-2.34986100	-4.17486100	-1.75902100
C	-0.66501100	-4.11590400	-0.39008500	H	-6.47505400	1.91774800	0.93965000
C	-0.53992300	-4.63799000	-2.77727100	C	5.61911900	-2.35036000	2.18888100
C	-1.40285900	-3.76927400	0.76984700	C	4.47452300	-1.69201200	2.63803400
C	0.76357500	-4.32052900	-0.29663400	C	3.86888700	-0.69743800	1.85648200
C	0.86935800	-4.82111200	-2.68263600	C	4.42613700	-0.36162300	0.62853200
H	-1.03346600	-4.76916000	-3.73663000	C	5.54747200	-1.07607000	0.17356400
C	-0.73622900	-3.60690800	2.00888400	C	6.16988200	-2.05755200	0.93509800
C	1.39715500	-4.19960700	0.94455600	H	6.08533800	-3.11106500	2.80864400
C	1.49705800	-4.67060400	-1.47483000	H	4.03638800	-1.95139800	3.59630500
H	1.43874100	-5.09045000	-3.56869300	H	2.95489100	-0.23127900	2.20134400
C	-1.41670100	-3.19182300	3.19960800	H	7.05050700	-2.57774700	0.57424800
C	0.68490600	-3.85568200	2.09728800	C	4.97477100	0.24816600	-1.61055600
H	2.46775700	-4.38350700	1.01637800	C	4.04670200	0.67506600	-0.43022100
H	2.57053400	-4.82419800	-1.38427100	N	5.87104800	-0.67746900	-1.13892500
C	-0.75630500	-3.08954600	4.39587200	C	6.89220400	-1.28378100	-1.98151500
H	-2.46143300	-2.91824400	3.12938600	H	6.71689800	-2.36609100	-2.02864700
C	1.33302300	-3.75001700	3.36875400	H	6.71605900	-0.87871500	-2.98371600
C	0.63363900	-3.38824800	4.48887000	C	8.31864000	-1.00990100	-1.53340800
H	-1.29324100	-2.76128300	5.28164400	C	9.30131800	-1.98773900	-1.72889000
H	2.39717400	-3.96802800	3.42108400	C	8.68657600	0.21862200	-0.97205100
H	1.13641200	-3.31526300	5.45025800	C	10.63042400	-1.74110300	-1.38030200
C	-6.02246200	2.78690700	1.40134500	H	9.02588000	-2.94852300	-2.15917100
C	-4.94353800	3.44325400	0.72606600	C	10.01346600	0.46383000	-0.61663200
C	-6.48762900	3.23502800	2.60979000	H	7.93045000	0.98019900	-0.80110500
C	-4.44324300	3.00306500	-0.52499500	C	10.98996800	-0.51337600	-0.82207300
C	-4.37790000	4.61652100	1.35412700	H	11.38124400	-2.51063500	-1.53807500
C	-5.91090500	4.37798800	3.23391100	H	10.28437000	1.41960300	-0.17606000
H	-7.30506600	2.71356200	3.10038000	H	12.02246700	-0.32104600	-0.54382800
C	-3.39579000	3.72093600	-1.15645900	O	4.93420500	0.67480800	-2.75806900
C	-3.36083600	5.32315200	0.70618900	C	3.92952500	4.93049100	3.07561400
C	-4.88856300	5.04826100	2.61889100	C	3.28268500	3.69246800	3.26014200
H	-6.29016200	4.71600800	4.19467100	C	3.37074300	2.68072200	2.31323100
C	-2.81774100	3.30931200	-2.40168400	C	4.12463900	2.88466500	1.13919000
C	-2.86330200	4.91335000	-0.53449900	C	4.75707400	4.15162600	0.98044400
H	-2.95548900	6.21890000	1.17319100	C	4.67329700	5.17549900	1.92993900
H	-4.44535800	5.92861200	3.07886200	H	3.84116400	5.70236900	3.83475300
C	-1.84054700	4.05014100	-3.01701400	H	2.69906300	3.52580300	4.16100300

H	2.85006500	1.74903500	2.48498000	C	4.62262300	2.23079100	-0.22703300
H	5.17123300	6.12854800	1.77123100	H	2.64667700	1.46332000	-0.61094600
C	5.22571600	2.92333900	-0.84103100	C	5.97345300	1.92382500	-0.04954100
C	4.44660700	2.10583600	-0.04692700	H	7.44108300	0.34368500	0.01980300
N	5.41404900	4.13848500	-0.23160500	H	4.28613500	3.26227900	-0.16360500
H	5.95254200	4.90034200	-0.61362600	H	6.69203200	2.71395500	0.15065000
H	5.64588800	2.72903200	-1.81608800	O	0.74029500	-0.96659300	-2.43672200
C	2.56222400	0.57703600	-0.92835400	C	-3.75983500	3.55743400	1.05562300
C	2.20189200	1.62225700	-1.94201900	C	-3.80159300	2.27460900	1.63648500
C	1.20520700	2.39196500	-1.47035100	C	-2.96990300	1.25276300	1.19754300
C	0.88437600	1.91760200	-0.14260200	C	-2.05347600	1.49593000	0.15518500
O	1.68335600	0.92562500	0.19977200	C	-2.05096000	2.79828900	-0.42308800
H	2.69707000	1.67305300	-2.90235000	C	-2.88660900	3.83235500	0.01216900
H	0.67364400	3.19722800	-1.95897800	H	-4.42449500	4.33604500	1.41983500
C	-0.22422900	2.26537300	0.66704100	H	-4.50775800	2.07674100	2.43828800
H	-0.17342600	1.93061300	1.70245500	H	-3.05791100	0.26625500	1.63106800
H	-0.57510500	3.28832400	0.52950200	H	-2.85366000	4.81346300	-0.45508500
H	-1.07581700	1.57209700	0.14693200	C	-0.52601300	1.56045700	-1.51317700
C	2.14517500	-0.82925700	-1.38374300	C	-1.05273500	0.71703900	-0.55757600
H	1.07825000	-0.83962800	-1.62302200	N	-1.11286400	2.80135600	-1.43259900
H	2.70779500	-1.11659700	-2.27641700	H	-0.90607700	3.58056800	-2.03724900
H	2.32727200	-1.55604100	-0.58944800	H	0.21507400	1.35591900	-2.27066700
14-an				C	-1.63629900	-1.81486500	-0.74552300
C	1.60826400	-1.30765600	3.33240000	C	-2.26877100	-1.55415500	-2.09204200
C	0.22245900	-1.20933300	3.45454300	C	-3.59498600	-1.45733400	-1.94967700
C	-0.58380200	-1.02260400	2.32218800	C	-3.93663300	-1.60067500	-0.53757700
C	0.00733300	-0.93253200	1.06742700	O	-2.75875900	-1.74375900	0.17072600
C	1.40258100	-1.06707500	0.96680000	H	-1.68134100	-1.48822000	-2.99770500
C	2.22242000	-1.24261400	2.07599200	H	-4.33243600	-1.30289400	-2.72803900
H	2.22306000	-1.44326800	4.21798200	C	-5.13718900	-1.61385700	0.05706700
H	-0.24132800	-1.27814400	4.43428700	H	-5.23974700	-1.74361400	1.12803900
H	-1.65892400	-0.97377500	2.42859800	H	-6.03572400	-1.48654100	-0.53459900
H	3.29966500	-1.32062400	1.97454000	C	-1.05753300	-3.23757200	-0.65672200
C	0.69346700	-0.92215200	-1.21407500	H	-1.85319500	-3.95913600	-0.86277700
C	-0.57532200	-0.72100500	-0.33287300	H	-0.26197500	-3.38475200	-1.39379800
N	1.78872800	-1.03231100	-0.38554800	H	-0.66120200	-3.43322900	0.34390200
C	3.13596700	-1.23635600	-0.89078100	15-ts-an			
H	3.52197600	-2.19051700	-0.50868000	C	1.83996400	-1.33187600	3.36926800
H	3.02183200	-1.33872300	-1.97550700	C	0.46965200	-1.12848400	3.55327800
C	4.11104800	-0.11735900	-0.55972600	C	-0.34665200	-0.74617600	2.48158300
C	5.46567400	-0.41818500	-0.37240400	C	0.21495100	-0.54283900	1.21549800
C	3.69743600	1.21782300	-0.48299000	C	1.59697600	-0.82496300	1.04326200
C	6.39342700	0.59467100	-0.12362300	C	2.41918900	-1.19578800	2.10093100
H	5.79795300	-1.45322900	-0.42330000	H	2.46437400	-1.61477600	4.21227300

H	0.02872900	-1.27301300	4.53564700	H	-5.10145300	-1.49394600	0.36005700
H	-1.41579900	-0.64561700	2.62788900	H	-5.42345000	-1.16003500	-1.44413500
H	3.47997500	-1.37022500	1.95256900	C	-0.45999100	-3.36030600	0.17247600
C	0.79204000	-0.34544300	-1.05295900	H	-0.86140600	-4.38150300	0.10770900
C	-0.34399800	-0.22771500	-0.09701100	H	0.54136600	-3.35683100	-0.26533400
N	1.91782100	-0.71311700	-0.31007300	H	-0.38648600	-3.09518300	1.22979200
C	3.21585900	-0.96003400	-0.91951200	17-an			
H	3.62972900	-1.89003900	-0.51100900	C	1.95539200	-1.75109800	3.16256900
H	3.00847600	-1.11844300	-1.98273900	C	0.60556500	-1.50417000	3.42567800
C	4.21157300	0.17462600	-0.74713900	C	-0.21593600	-0.90815800	2.46113900
C	5.44747300	-0.03969200	-0.12943800	C	0.31703700	-0.53108700	1.21856300
C	3.90779500	1.45413900	-1.23382200	C	1.68078700	-0.85976400	0.95690800
C	6.36769400	1.00341500	0.00661900	C	2.50537800	-1.44191600	1.91125700
H	5.69620500	-1.03079600	0.24557000	H	2.58454500	-2.20092300	3.92565100
C	4.82273900	2.49663200	-1.09615400	H	0.18253800	-1.78022400	4.38766100
H	2.95345500	1.62166500	-1.72628900	H	-1.26946800	-0.77148200	2.67189700
C	6.05559000	2.27472500	-0.47458200	H	3.54926000	-1.64788600	1.69712100
H	7.32366600	0.82148600	0.49081100	C	0.84479800	-0.01853000	-1.00568900
H	4.57629200	3.48412400	-1.47766400	C	-0.23384900	0.04135100	0.00544600
H	6.76759900	3.08890600	-0.36834700	N	1.97471600	-0.54422700	-0.36597100
O	0.81994100	-0.16384800	-2.27393700	C	3.23273400	-0.77317100	-1.05701700
C	-4.37152200	3.18280600	1.32137900	H	3.59686900	-1.77877400	-0.81294300
C	-3.46488500	2.58763100	2.21689500	H	2.98274800	-0.75180700	-2.12281000
C	-2.46663900	1.72667700	1.77147400	C	4.30704200	0.25838000	-0.75473800
C	-2.35719100	1.42959600	0.40035900	C	5.55056800	-0.12561800	-0.24400000
C	-3.26656600	2.07921300	-0.47960900	C	4.06821300	1.61591800	-1.01211700
C	-4.27540400	2.94121800	-0.04401200	C	6.54174700	0.82605300	0.01177900
H	-5.14276800	3.84993100	1.69644300	H	5.74876800	-1.17755400	-0.04669100
H	-3.53750700	2.81199100	3.27755900	C	5.05395400	2.56717000	-0.75458400
H	-1.76109300	1.32123800	2.48363300	H	3.10724300	1.91655300	-1.42143700
H	-4.95178300	3.41530800	-0.75086700	C	6.29410400	2.17516500	-0.24087600
C	-1.83321900	0.89829900	-1.75120500	H	7.50279200	0.51213400	0.41097100
C	-1.44557100	0.64283300	-0.43008700	H	4.85704100	3.61656800	-0.95834100
N	-2.91624500	1.73391200	-1.77287800	H	7.06153200	2.91822700	-0.04057700
H	-3.34351800	2.10346700	-2.60770200	O	0.84796800	0.32667700	-2.19452100
H	-1.32763400	0.59754400	-2.65309800	C	-4.68745500	2.68144100	1.66677800
C	-1.35507300	-2.42388500	-0.56459100	C	-3.71979800	2.12029400	2.51899600
C	-1.48442600	-2.26367800	-1.96625800	C	-2.61301200	1.44924200	2.00773400
C	-2.74433900	-1.78799200	-2.21390400	C	-2.45681100	1.31488000	0.61688200
C	-3.46419800	-1.76754700	-0.96047900	C	-3.43433700	1.92392200	-0.21463600
O	-2.57273600	-2.18824400	0.02379400	C	-4.55012600	2.59846500	0.28554100
H	-0.68039800	-2.39836500	-2.67557600	H	-5.54299800	3.20070200	2.08989000
H	-3.18217100	-1.53435200	-3.16989900	H	-3.83024000	2.22310700	3.59477400
C	-4.73899600	-1.45895200	-0.65984400	H	-1.86032000	1.07261500	2.68718100

H	-5.27703500	3.05368300	-0.38219600	C	-6.31326900	-2.15990800	-0.23568800
C	-1.83217400	1.10499600	-1.57671300	H	-7.51644300	-0.48877300	0.40557500
C	-1.42444600	0.76299100	-0.26078900	H	-4.88057100	-3.61068200	-0.94292800
N	-3.01773300	1.78518900	-1.52997700	H	-7.08434300	-2.89876900	-0.03390000
H	-3.47264800	2.20489800	-2.32542500	O	-0.85003500	-0.31382100	-2.20395900
H	-1.22792600	1.05503900	-2.46639600	C	4.62266400	-2.74188500	1.66583600
C	-1.58908300	-2.53414300	-0.82974400	C	3.65447000	-2.17705200	2.51484700
C	-1.36930600	-2.03972500	-2.10387700	C	2.56970000	-1.47499400	1.99818200
C	-2.49046200	-1.28095800	-2.44822400	C	2.43839200	-1.31547800	0.60774600
C	-3.45252100	-1.44348000	-1.39507600	C	3.41466100	-1.92814000	-0.22296600
O	-2.82929100	-2.18432100	-0.38773500	C	4.51004800	-2.63144500	0.28410400
H	-0.46019000	-2.15727500	-2.67498000	H	5.46153100	-3.28545800	2.09198700
H	-2.70493200	-0.82552900	-3.40413100	H	3.74769800	-2.30000900	3.59003000
C	-4.73146000	-1.03448100	-1.25290900	H	1.81494800	-1.09038300	2.67121500
H	-5.29172800	-1.24329700	-0.35012800	H	5.23972700	-3.08831500	-0.37934400
H	-5.22149800	-0.49938600	-2.05631900	C	1.85923800	-1.03162700	-1.60109900
C	-0.82120100	-3.46629600	0.02909500	C	1.42289800	-0.73642000	-0.26955800
H	-1.34942800	-4.42440600	0.12447400	N	3.02368000	-1.76069100	-1.54073100
H	0.16650600	-3.65077200	-0.39997700	H	3.48136600	-2.18028900	-2.33431700
H	-0.69179500	-3.05583200	1.03816600	H	1.22327400	-1.04562500	-2.47108800
18-ts-an				C	1.63735700	2.55940900	-0.87141400
C	-1.95181300	1.76994400	3.15170000	C	1.42736300	1.97888600	-2.09998700
C	-0.59999800	1.53032600	3.41113100	C	2.53314100	1.14311400	-2.35721700
C	0.21912300	0.92835200	2.44800700	C	3.49699300	1.40841400	-1.31670700
C	-0.31923200	0.54078200	1.21228200	O	2.86407300	2.22057100	-0.37301300
C	-1.68354000	0.86179700	0.95259900	H	0.53121400	2.07141100	-2.69532800
C	-2.50660500	1.44876900	1.90565600	H	2.79377100	0.70030500	-3.30800600
H	-2.57914200	2.22388100	3.91387400	C	4.77743800	1.02774900	-1.14590000
H	-0.17395100	1.81592500	4.36896500	H	5.33630400	1.31426600	-0.26344700
H	1.27434500	0.79538500	2.65435500	H	5.27146100	0.43025600	-1.90133100
H	-3.55190700	1.65021600	1.69428900	C	0.85280400	3.52834300	-0.06838500
C	-0.84818900	0.02511800	-1.01354200	H	1.40289800	4.47161600	0.04339400
C	0.23076300	-0.03582700	-0.00182000	H	-0.10560600	3.73362700	-0.55114600
N	-1.98037300	0.53800900	-0.36888500	H	0.65990400	3.13442200	0.93748300
C	-3.23814700	0.77191900	-1.05882800	19-an			
H	-3.59715800	1.77962900	-0.81563600	C	2.03746400	-0.23562700	3.67546000
H	-2.98954400	0.74815400	-2.12490500	C	0.70026900	0.13251800	3.84386200
C	-4.31687600	-0.25392500	-0.75351500	C	-0.14942000	0.25693500	2.73872900
C	-5.55997800	0.13767500	-0.24751100	C	0.34845200	0.03112400	1.45200900
C	-4.08318600	-1.61359000	-1.00393000	C	1.69093100	-0.40596100	1.31536600
C	-6.55578200	-0.80860800	0.01018900	C	2.54737900	-0.52536600	2.40347200
H	-5.75417300	1.19133800	-0.05555700	H	2.69008100	-0.31585800	4.54048400
C	-5.07353600	-2.55953300	-0.74450500	H	0.31153800	0.31868000	4.84092800
H	-3.12246600	-1.92034100	-1.40937000	H	-1.19631400	0.49535400	2.89030900

H	3.58053600	-0.83118700	2.27553800	H	-1.92699800	-5.09222300	0.69262400
C	0.78249500	-0.56223300	-0.78999000	C	-4.81899300	-1.19291100	-0.20116400
C	-0.26313600	-0.01194600	0.12535200	H	-5.25127000	-0.45722300	-0.86589600
N	1.93523800	-0.72375400	-0.02245800	H	-5.37928700	-1.49739400	0.67624900
C	3.17991900	-1.23802200	-0.57465500	20-ts-an			
H	3.56426400	-2.02077200	0.09028400	C	2.35235800	-2.69291900	-2.68314000
H	2.90334200	-1.70602900	-1.52452200	C	1.03602300	-3.15966300	-2.65638100
C	4.24149000	-0.17589400	-0.80461900	C	0.06186100	-2.50395800	-1.89485600
C	5.49456200	-0.26561100	-0.19093200	C	0.40647000	-1.38040900	-1.13619800
C	3.97983400	0.90284100	-1.66135600	C	1.73775000	-0.89165800	-1.23183500
C	6.47279100	0.70566500	-0.42111800	C	2.71623400	-1.53944800	-1.97754700
H	5.71083100	-1.10322600	0.46953900	H	3.10252800	-3.21852900	-3.26764200
C	4.95274000	1.87449800	-1.88968000	H	0.76022300	-4.03633000	-3.23569200
H	3.01172900	0.96853800	-2.15118500	H	-0.96307800	-2.85376900	-1.92970500
C	6.20233400	1.77932100	-1.26924200	H	3.73442500	-1.16576000	-2.01018600
H	7.44164100	0.62314400	0.06451700	C	0.60500200	0.65956500	0.02624000
H	4.73873800	2.70601500	-2.55616700	C	-0.34543600	-0.44140000	-0.30431400
H	6.95979600	2.53767300	-1.44884900	N	1.83920600	0.30626600	-0.52759100
O	0.75044800	-0.76767700	-2.00583100	C	3.00818800	1.16728500	-0.44642900
C	-4.01115900	3.78522600	0.32424700	H	3.44711200	1.26953700	-1.44661600
C	-3.05548100	3.53836100	1.32489900	H	2.62244500	2.14629500	-0.14450700
C	-2.19106300	2.45394200	1.22307800	C	4.06084000	0.69231900	0.54109800
C	-2.27952300	1.58921100	0.11703100	C	5.37971400	0.46719900	0.13509600
C	-3.24077900	1.87086800	-0.89185500	C	3.72261100	0.49701200	1.88774000
C	-4.11202000	2.96258400	-0.79303400	C	6.34766400	0.04944300	1.05280800
H	-4.67951200	4.63702700	0.41958200	H	5.65506800	0.62191100	-0.90650400
H	-2.98541900	4.20412200	2.17981100	C	4.68530400	0.07708600	2.80411400
H	-1.43364300	2.30059000	1.98053800	H	2.70155300	0.68296600	2.21073500
H	-4.84290200	3.16067700	-1.57220500	C	6.00137600	-0.14913000	2.38919200
C	-2.05749000	0.02359200	-1.67394200	H	7.36815400	-0.12368200	0.72097400
C	-1.44216000	0.50375900	-0.36365500	H	4.41038400	-0.07091000	3.84528400
N	-3.15711300	0.95827200	-1.91839500	H	6.75070000	-0.47711100	3.10480900
H	-3.36714300	1.24317400	-2.86494600	O	0.43272800	1.68312300	0.69133400
H	-1.32015700	0.03239800	-2.48254400	C	-4.51819600	-3.37781500	1.55480900
C	-3.61054500	-1.69735200	-0.44685900	C	-3.45886900	-3.89003300	0.78692200
C	-2.64373200	-1.45154800	-1.60207200	C	-2.43448300	-3.06211000	0.33555500
C	-1.63276200	-2.53879900	-1.35779900	C	-2.45782900	-1.68950900	0.63801900
C	-1.91813400	-3.14753600	-0.20186800	C	-3.51227600	-1.21369500	1.46803500
O	-3.06046100	-2.65007900	0.40577900	C	-4.55356100	-2.03340800	1.91171200
H	-3.16356400	-1.57788200	-2.56104600	H	-5.31156500	-4.04088200	1.88900200
H	-0.78056100	-2.73760300	-1.98931000	H	-3.43430900	-4.94884500	0.54578100
C	-1.24634700	-4.24465100	0.54649600	H	-1.61199400	-3.49138200	-0.22018600
H	-0.36230300	-4.59086900	0.00514300	H	-5.35270500	-1.63612100	2.53210800
H	-0.93767900	-3.89862500	1.54053900	C	-2.18107500	0.57204300	1.03130100

C	-1.55894100	-0.56047800	0.39403200	H	-3.76720300	0.87542400	-0.83081600
N	-3.27144400	0.11233800	1.76198500	H	-4.24497900	3.19024300	0.56316800
H	-3.91493500	0.71562100	2.25004500	C	-2.20307200	5.27457600	-0.16555600
H	-1.62954100	1.43576400	1.36915500	H	-2.99818700	5.66875300	0.47276300
C	-1.94236800	1.93074500	-1.49664200	H	-1.24354600	5.40360700	0.35052500
C	-3.05989700	1.67158600	-0.63604800	H	-2.16216400	5.87146200	-1.08491800
C	-3.40887700	2.96229600	-0.08435500	C	-1.22357600	1.09801400	-2.29400300
C	-2.44566800	3.83958800	-0.47089200	H	-1.61054100	0.12326000	-2.55217500
O	-1.53674400	3.24577900	-1.30458700	H	-0.35367100	1.45828500	-2.83099700

6. X-ray Crystal Data for Product 3a

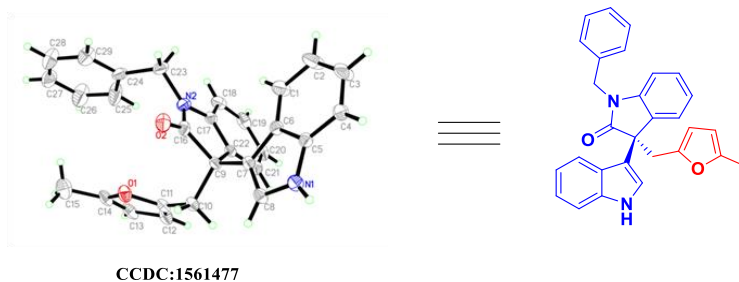


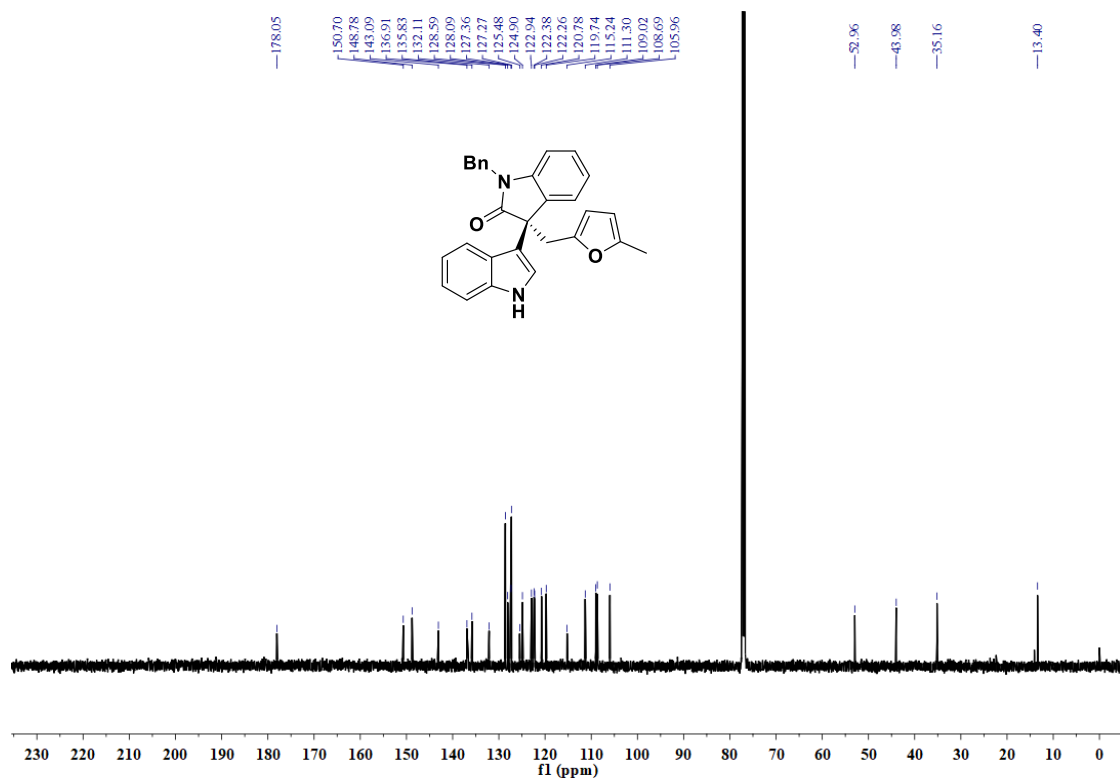
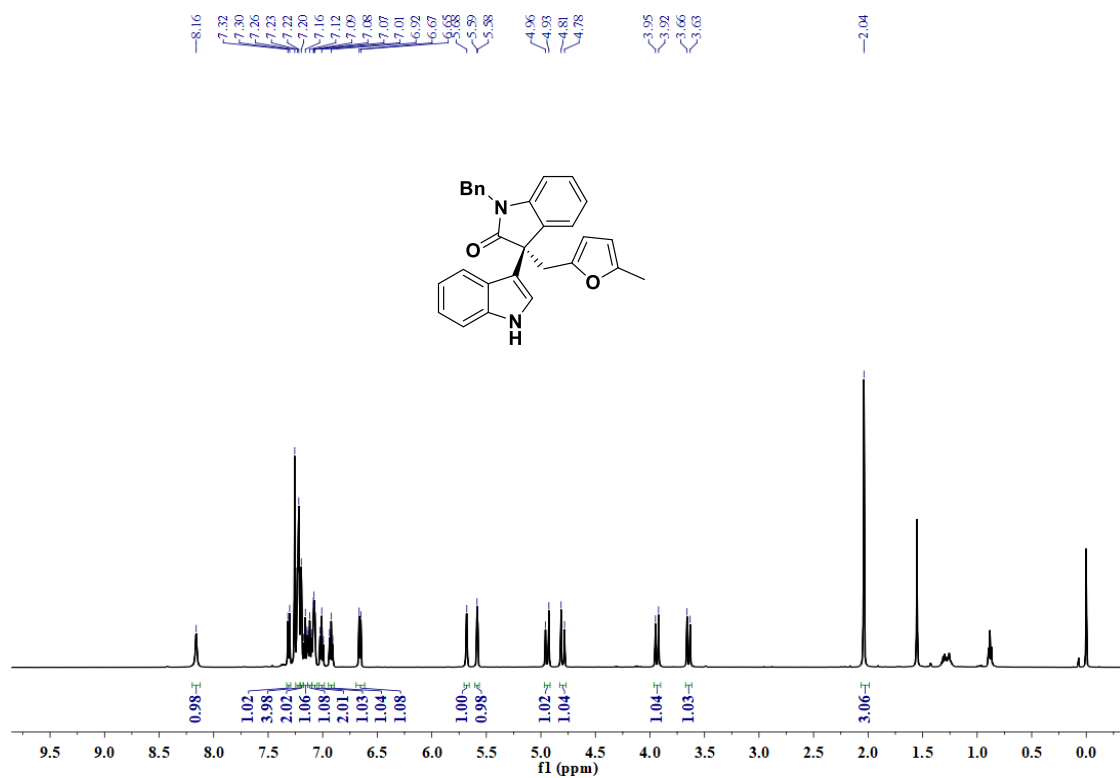
Table 1. Crystal data and structure refinement for **3a**

Identification code	3a
Empirical formula	C ₂₉ H ₂₄ N ₂ O ₂
Formula weight	432.50
Temperature	123.2(2) K
Wavelength	1.54184 Å
Crystal system, space group	Orthorhombic, P2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 9.1297(8) Å alpha = 90 deg. b = 10.3260(9) Å beta = 90 deg. c = 24.1270(18) Å gamma = 90 deg.
Volume	2274.5(3) Å ³
Z,	4
Calculated density	1.263 Mg/m ³
Absorption coefficient	0.629 mm ⁻¹
F(000)	912
Crystal size	0.12 x 0.11 x 0.11 mm
Theta range for data collection	3.66 to 67.24 deg.
Limiting indices	-10 ≤ h ≤ 10, -12 ≤ k ≤ 6, -18 ≤ l ≤ 28
Reflections collected / unique	4857 / 3406 [R(int) = 0.0316]
Completeness to theta = 67.24	100.0 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9340 and 0.9283
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	3406 / 0 / 299
Goodness-of-fit on F ²	1.040
Final R indices [I > 2sigma(I)]	R1 = 0.0574, wR2 = 0.1248

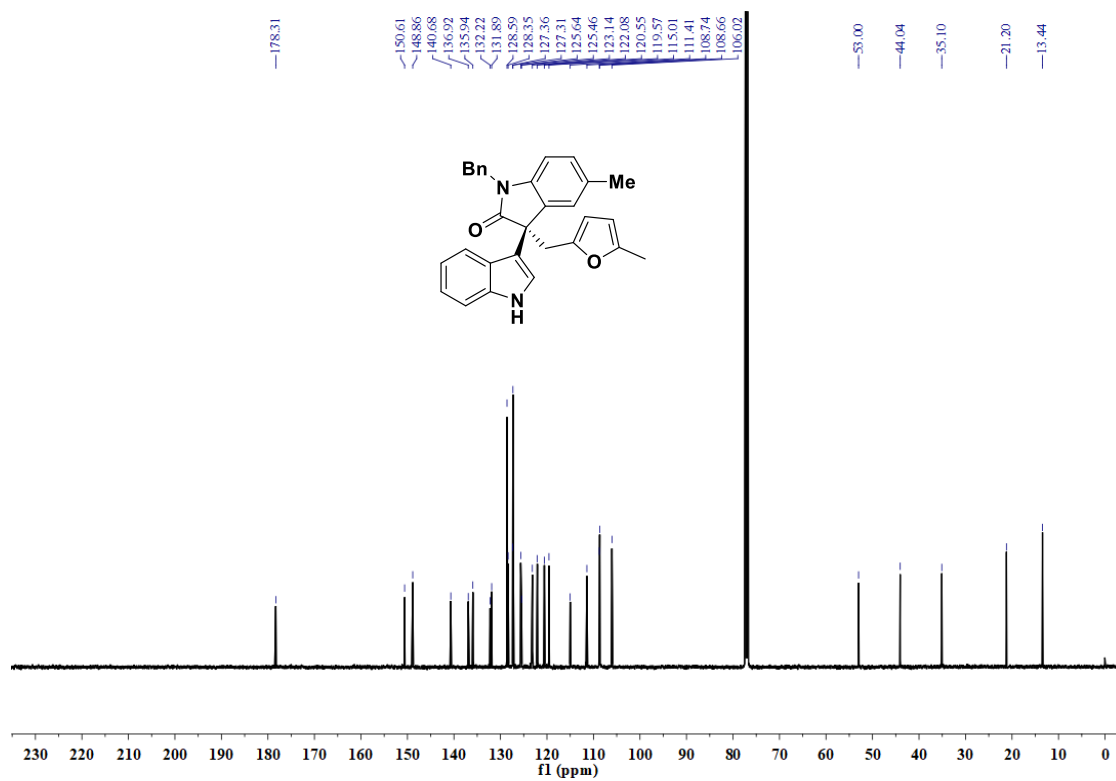
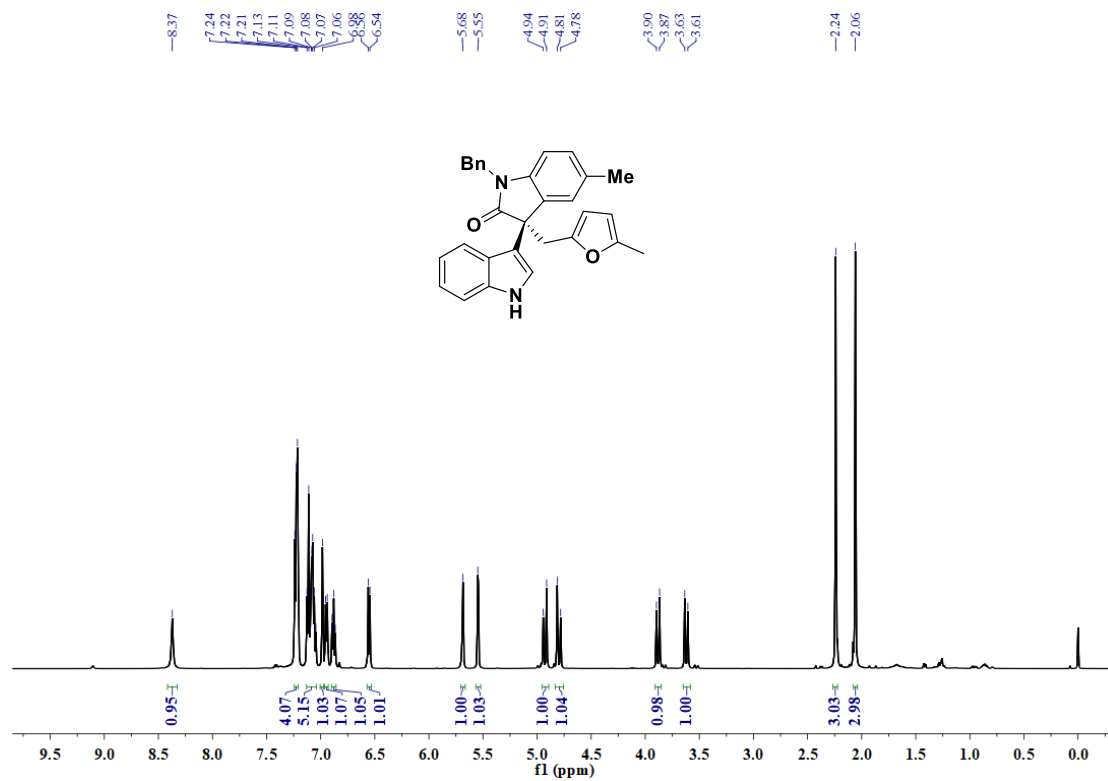
R indices (all data)	$R_1 = 0.0767$, $wR_2 = 0.1388$
Absolute structure parameter	$-0.4(5)$
Largest diff. peak and hole	0.164 and -0.222 e.Å^{-3}

7. NMR Spectra for All Products

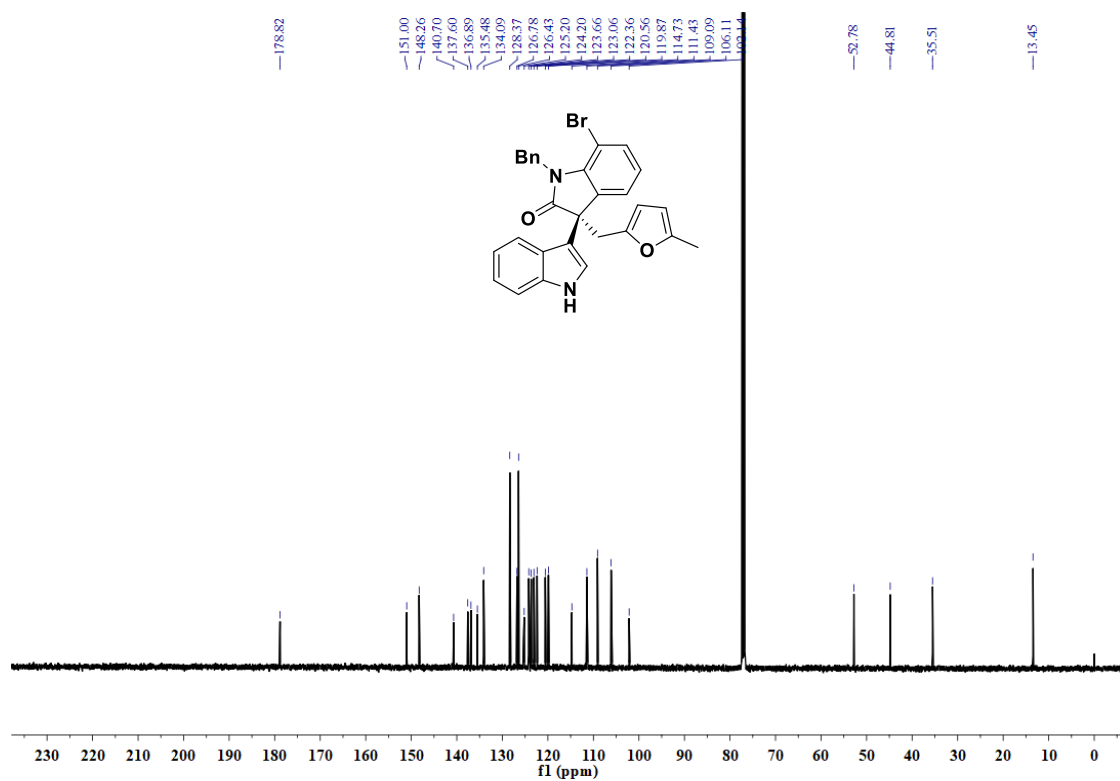
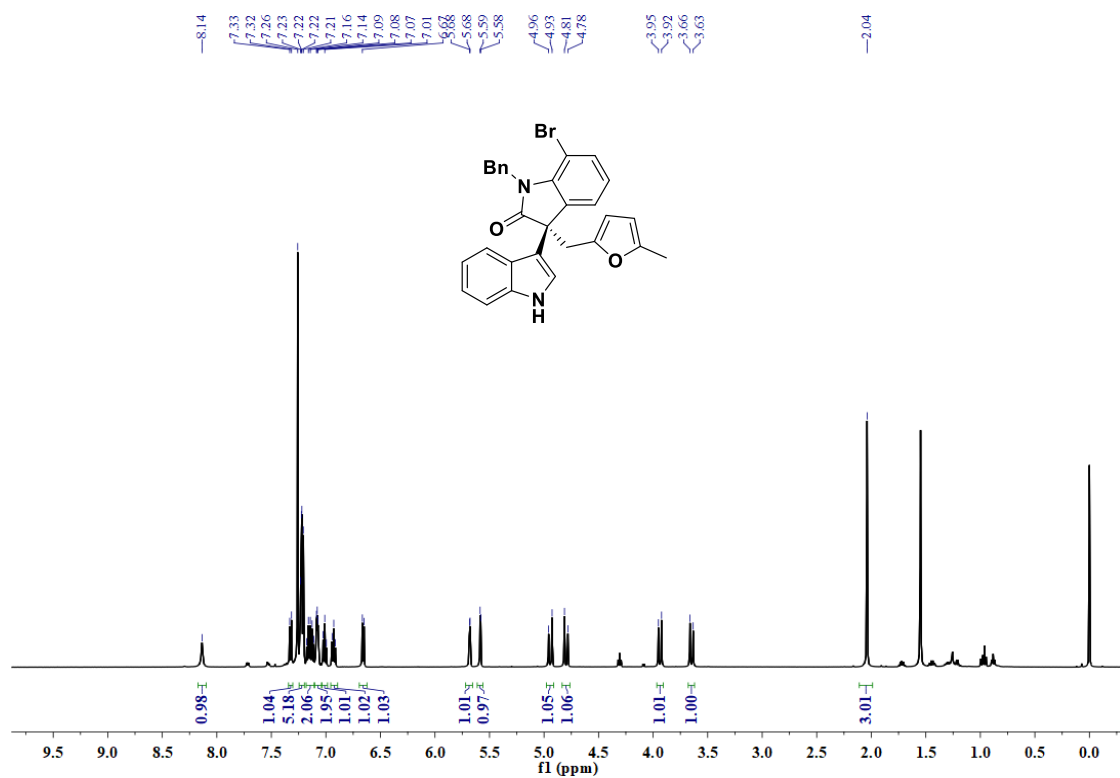
(R)-1-benzyl-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3a)



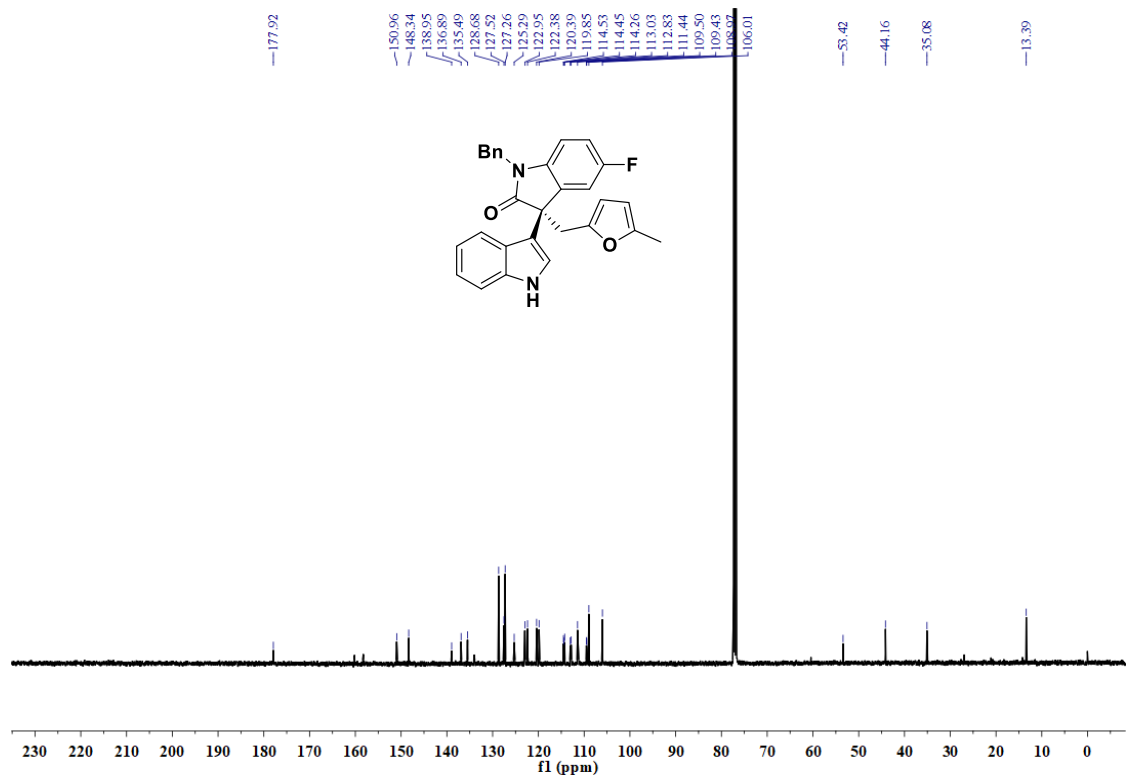
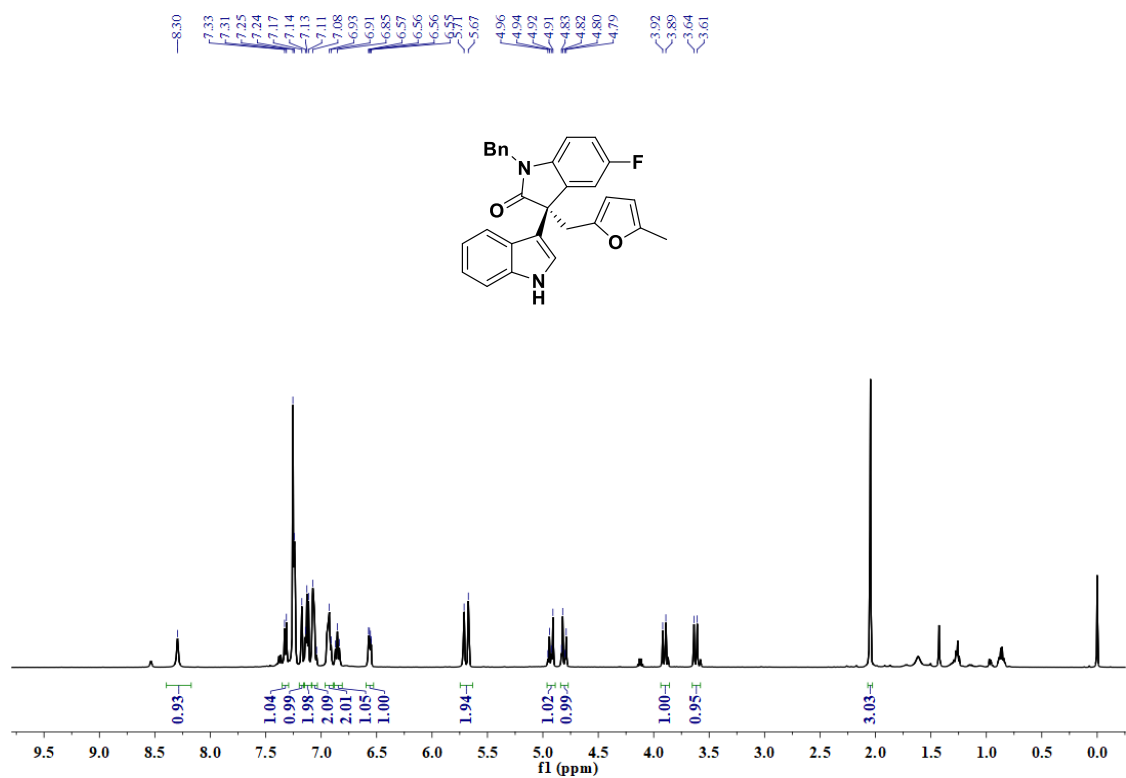
(R)-1-benzyl-3-(1H-indol-3-yl)-5-methyl-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3b)



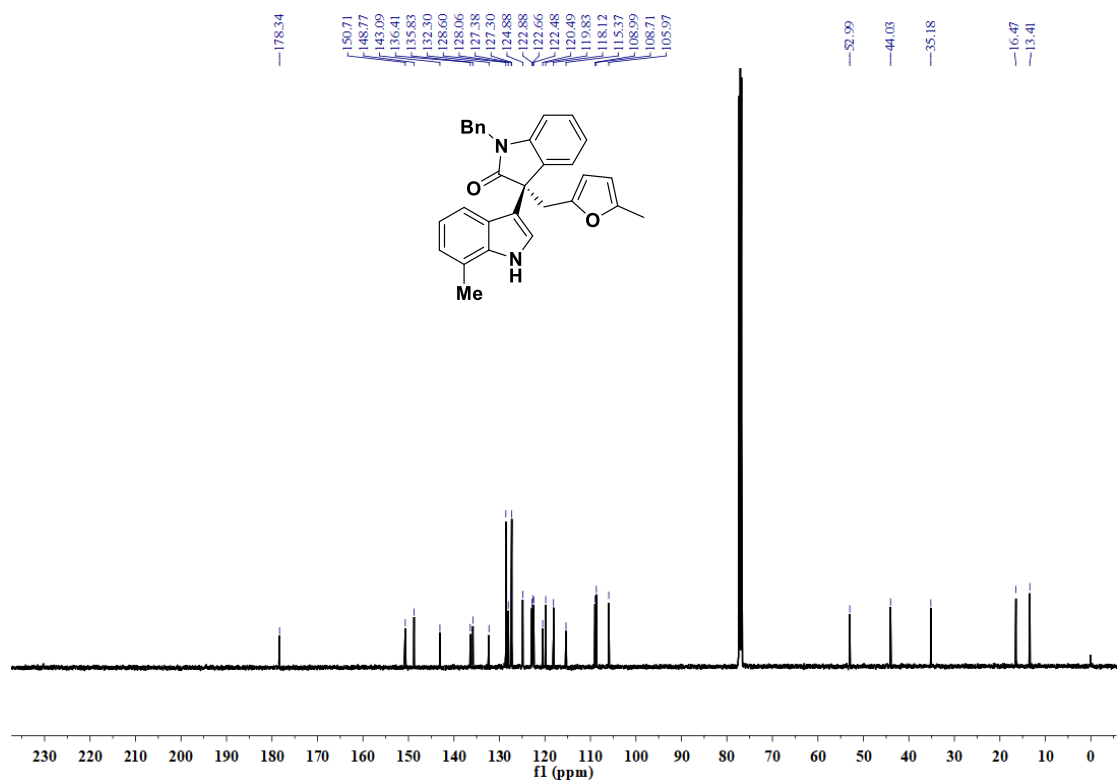
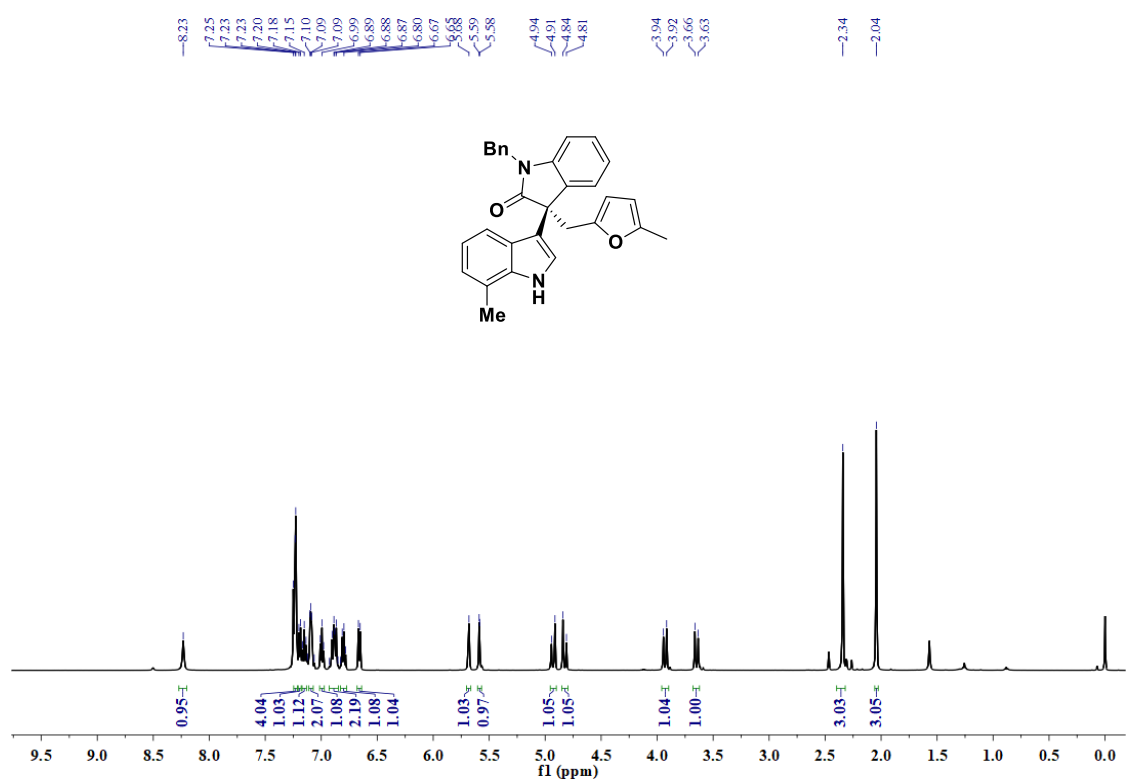
(R)-1-benzyl-7-bromo-3-((1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3c)



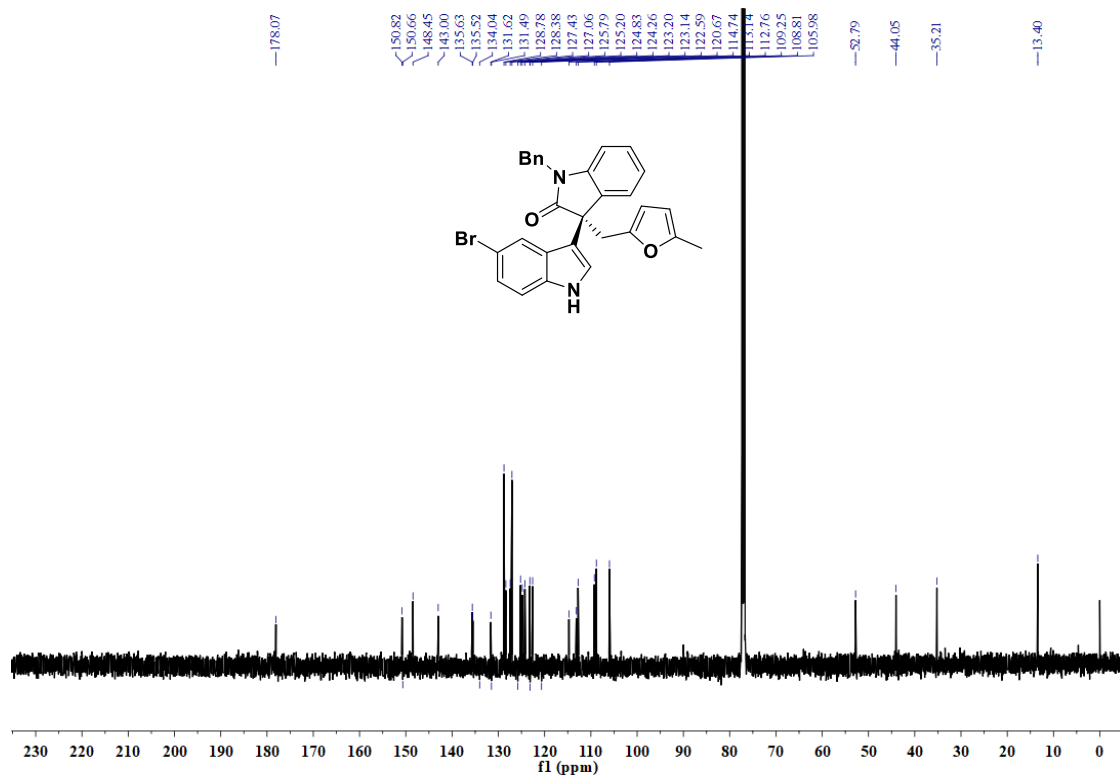
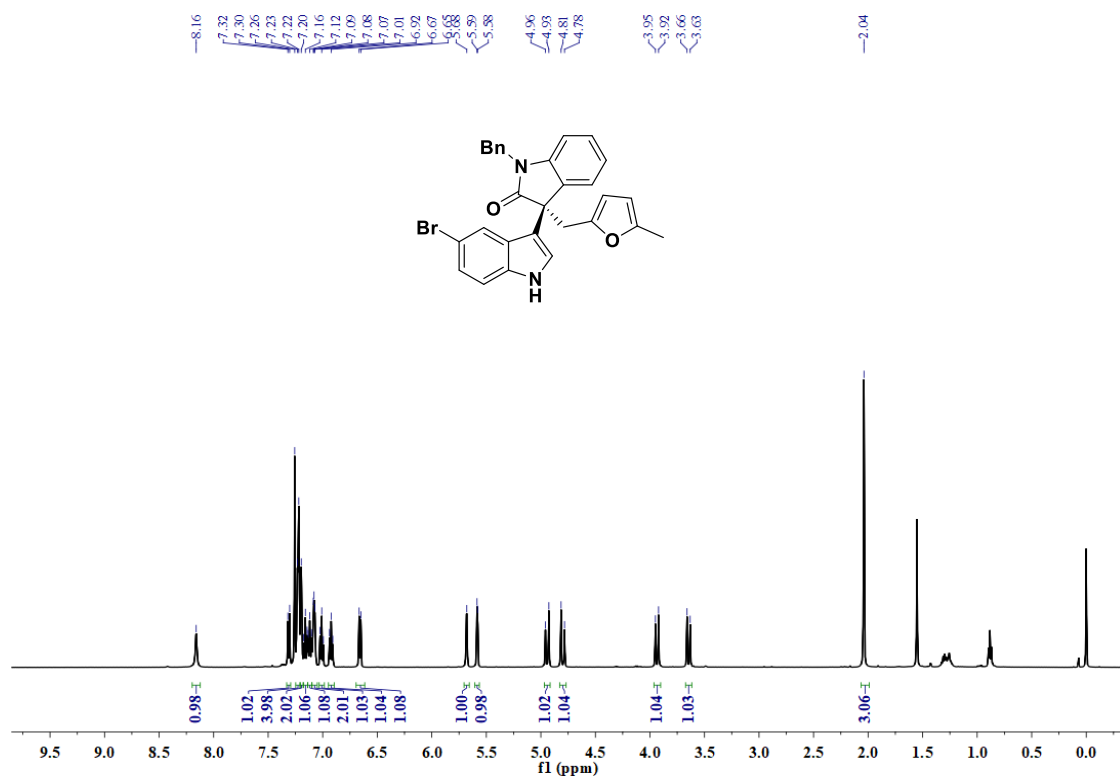
(R)-1-benzyl-5-fluoro-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3d)



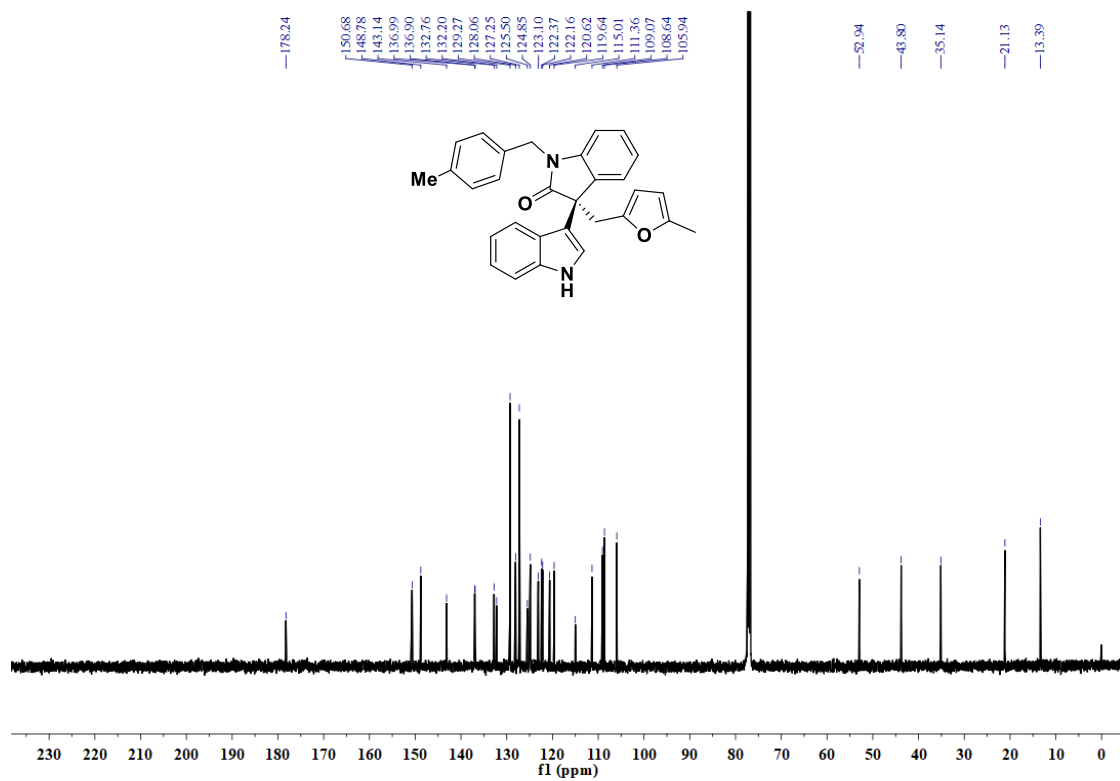
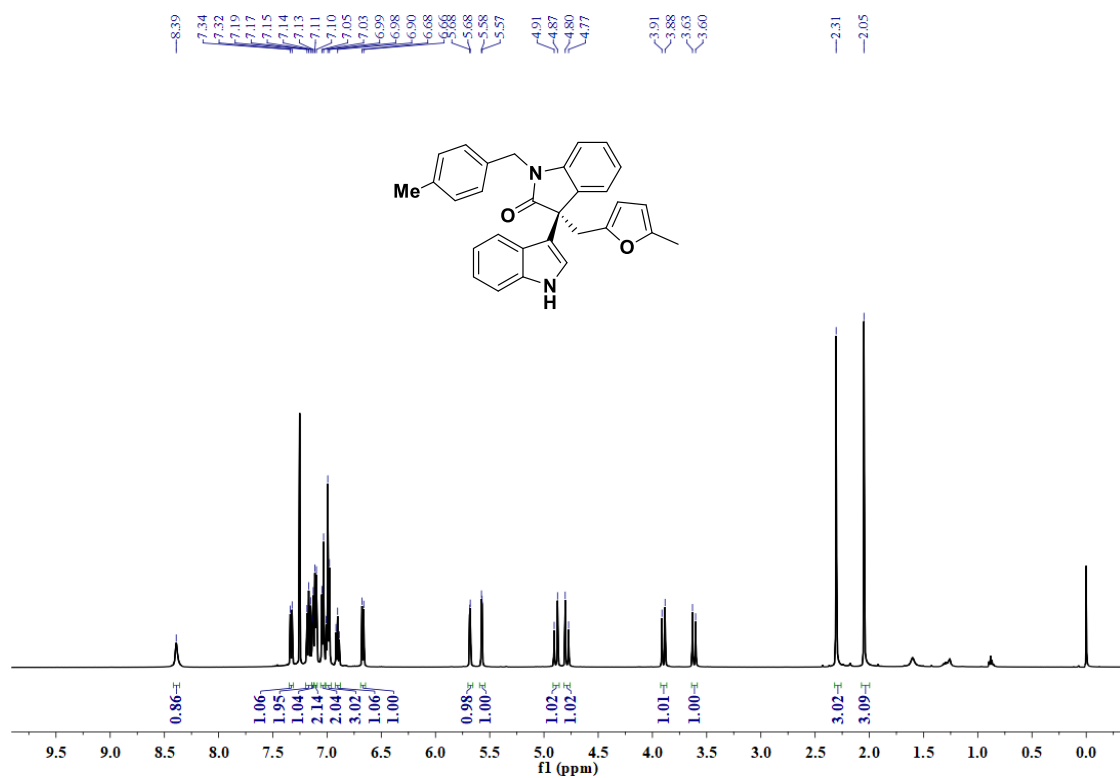
(R)-1-benzyl-3-(7-methyl-1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3e)



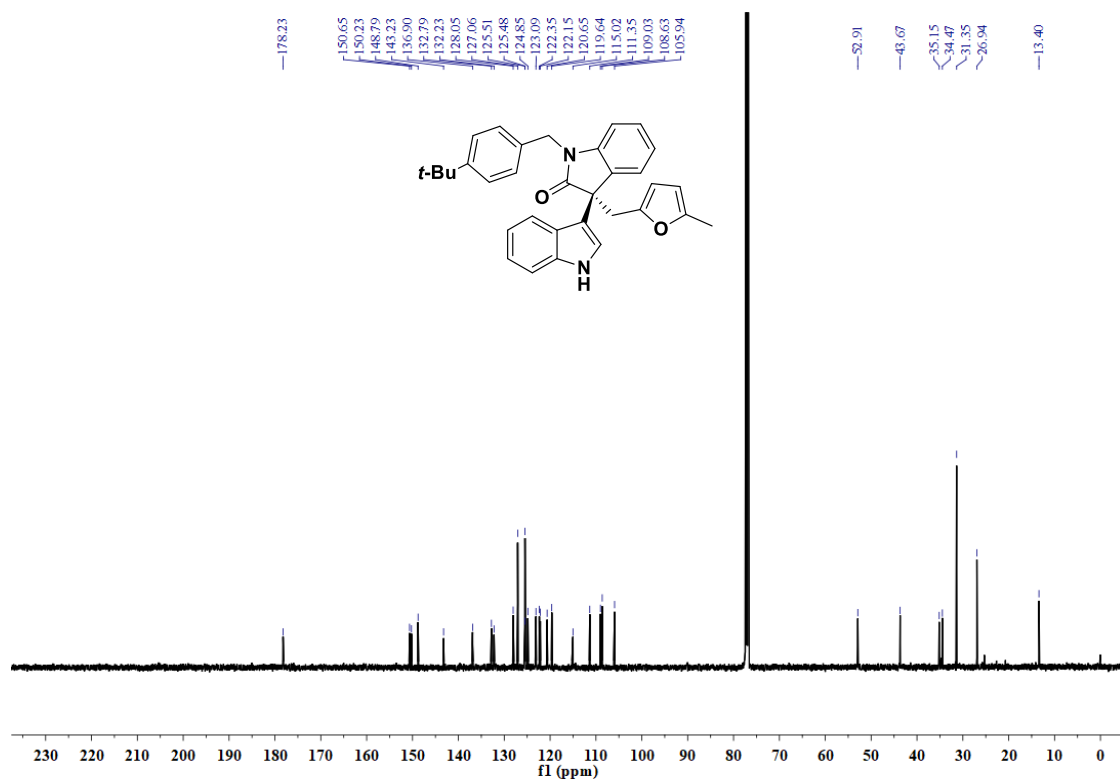
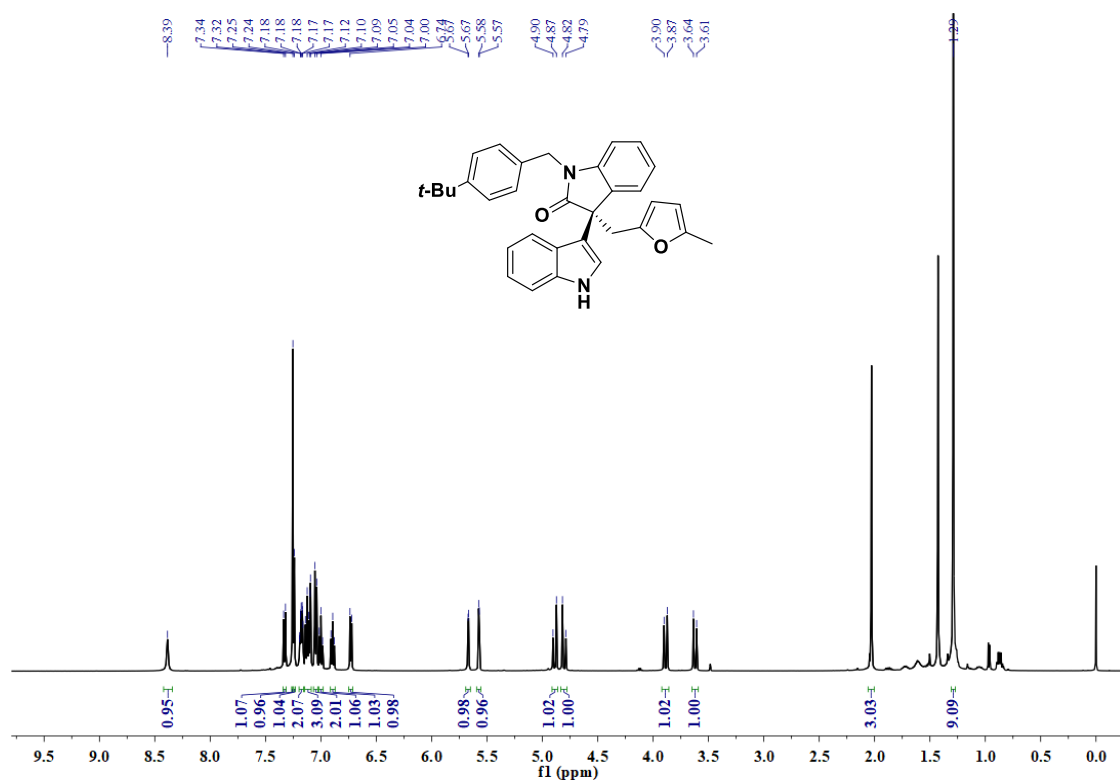
(R)-1-benzyl-3-(5-bromo-1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3f)



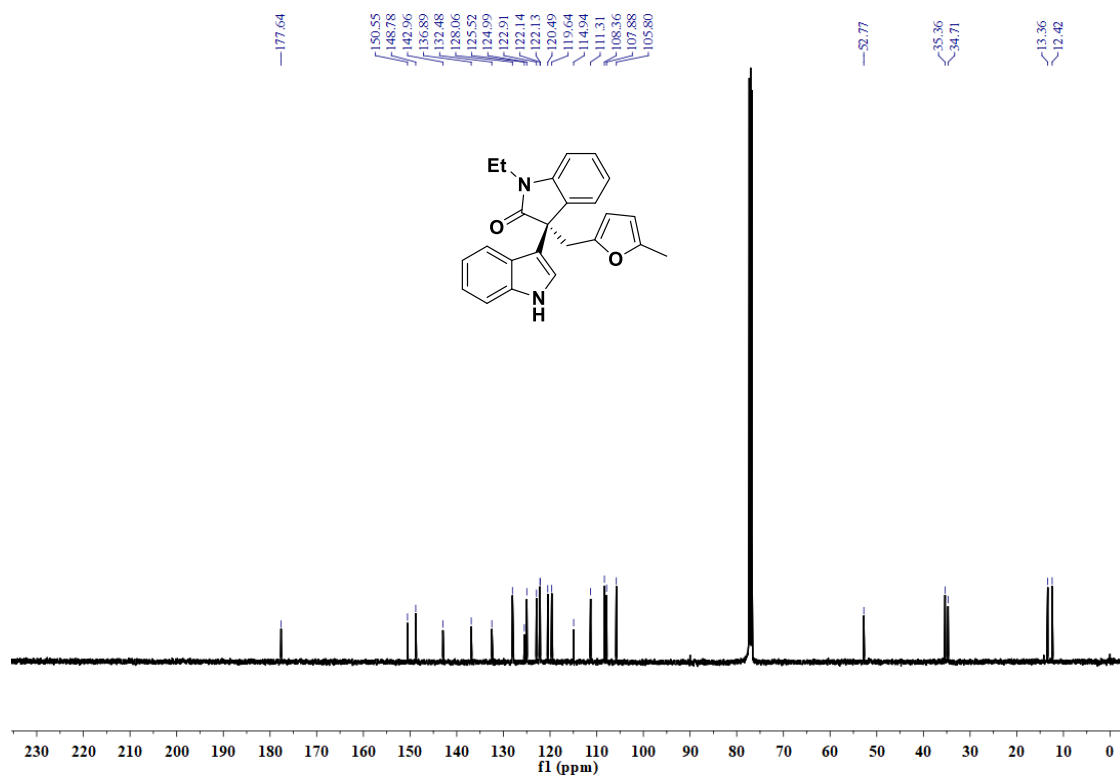
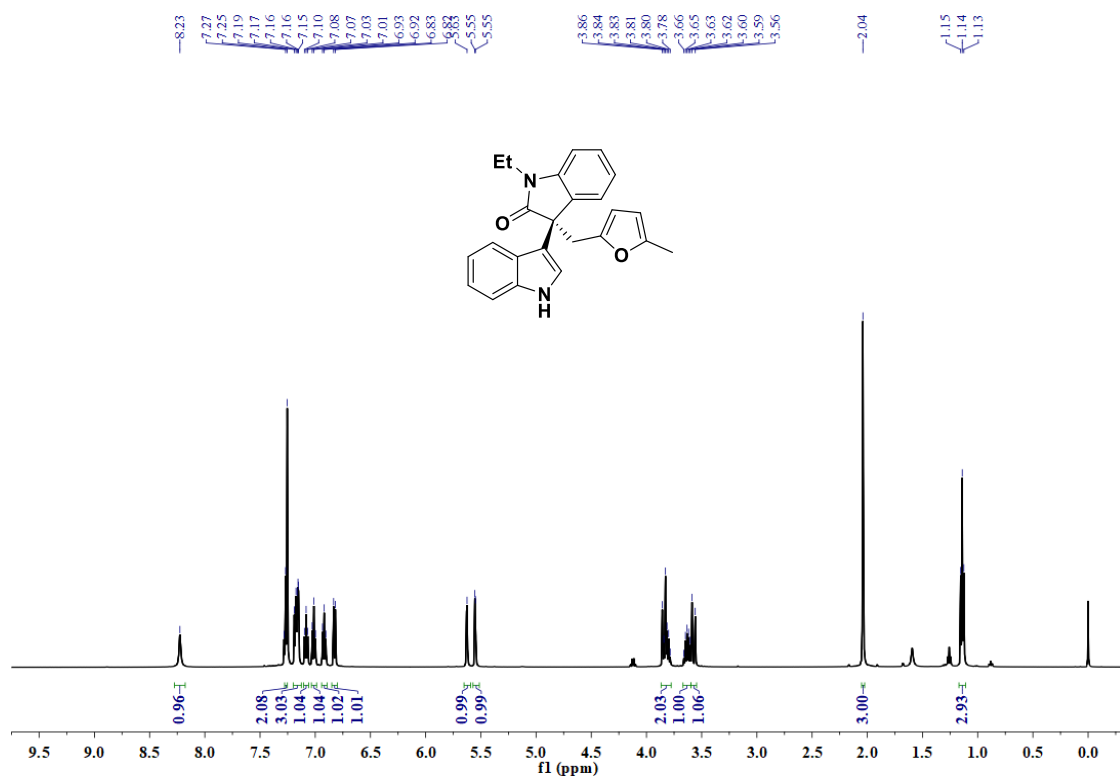
(R)-3-(1H-indol-3-yl)-1-(4-methylbenzyl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3g)



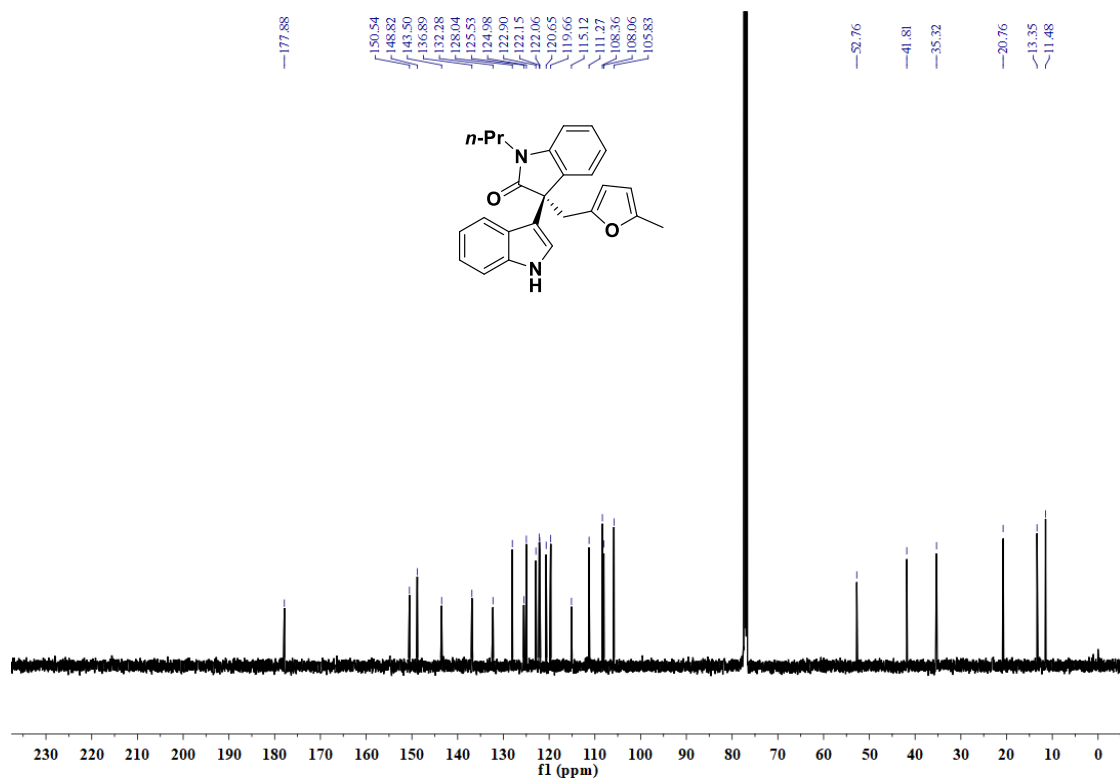
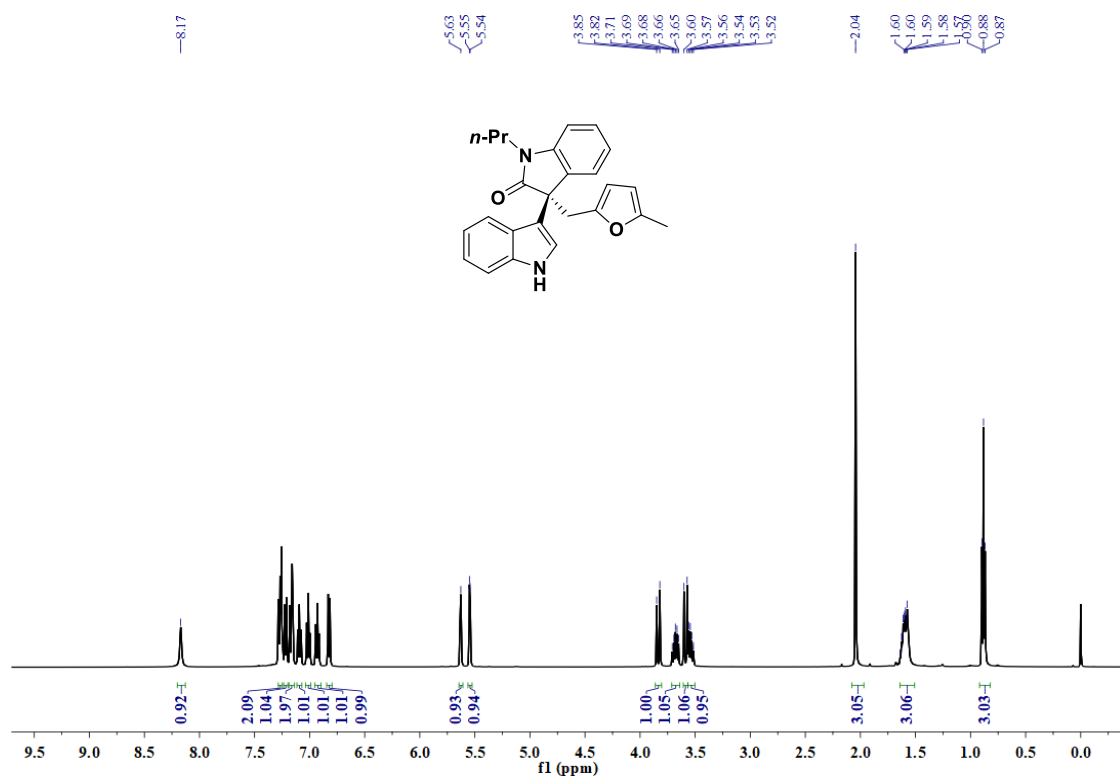
(R)-1-(4-(tert-butyl)benzyl)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3h)



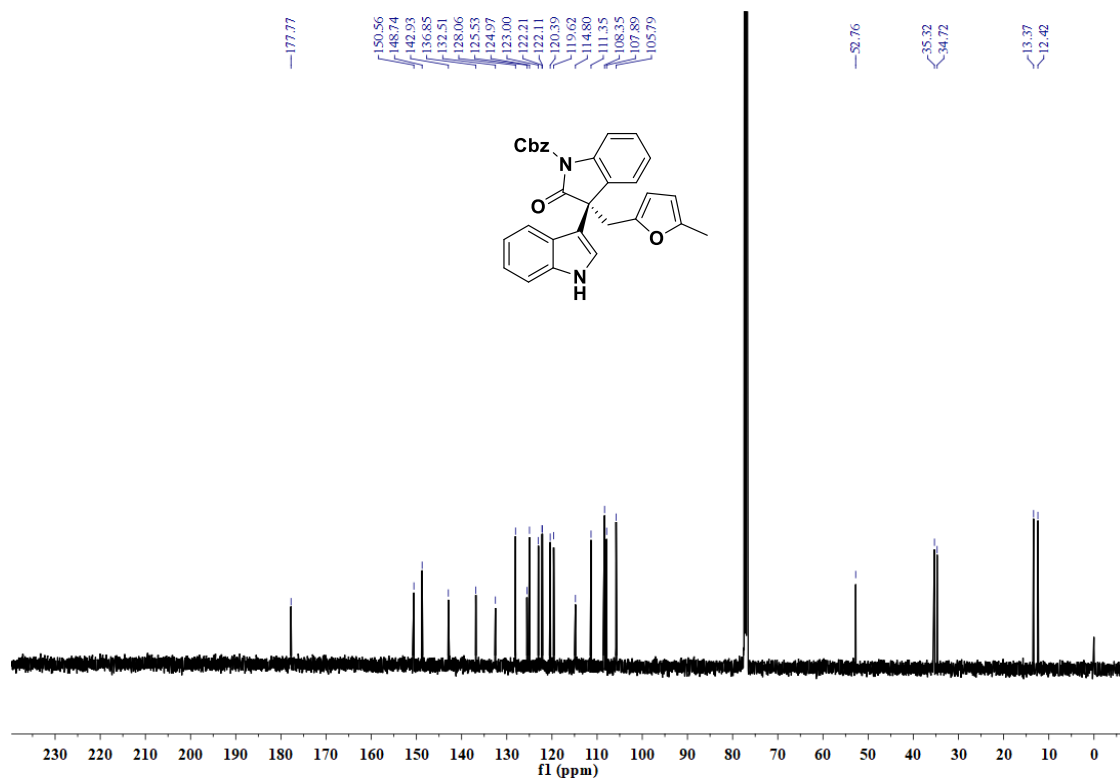
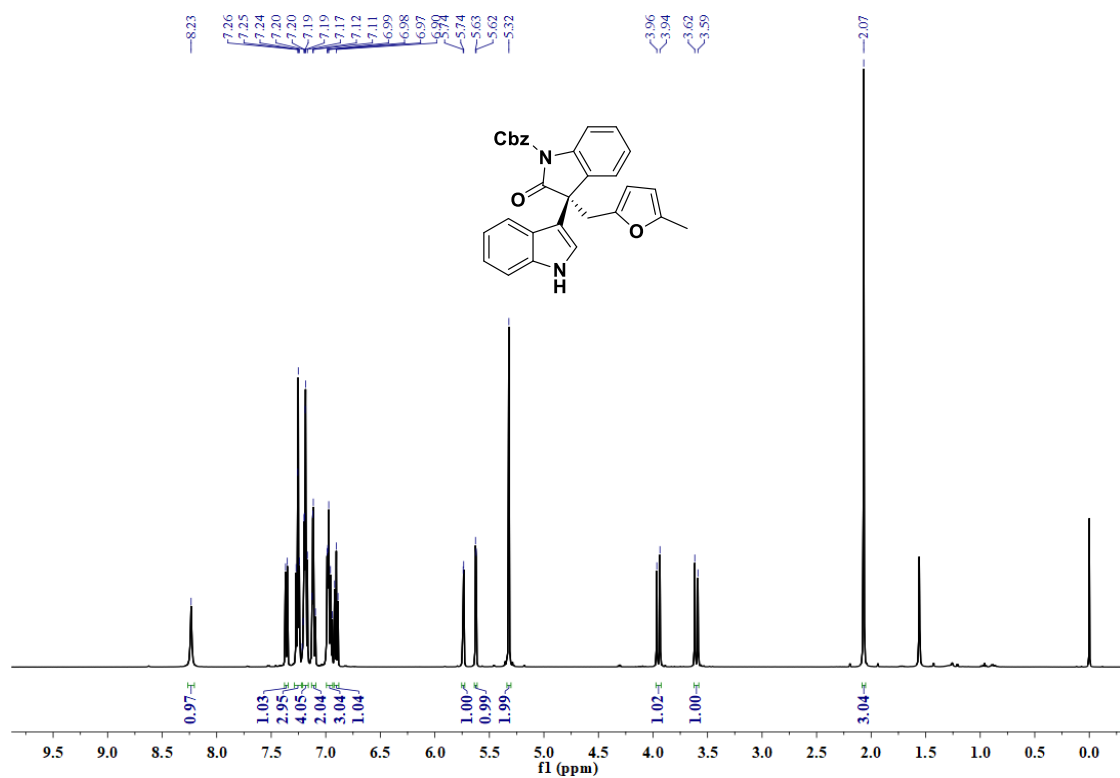
(R)-1-ethyl-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3i)



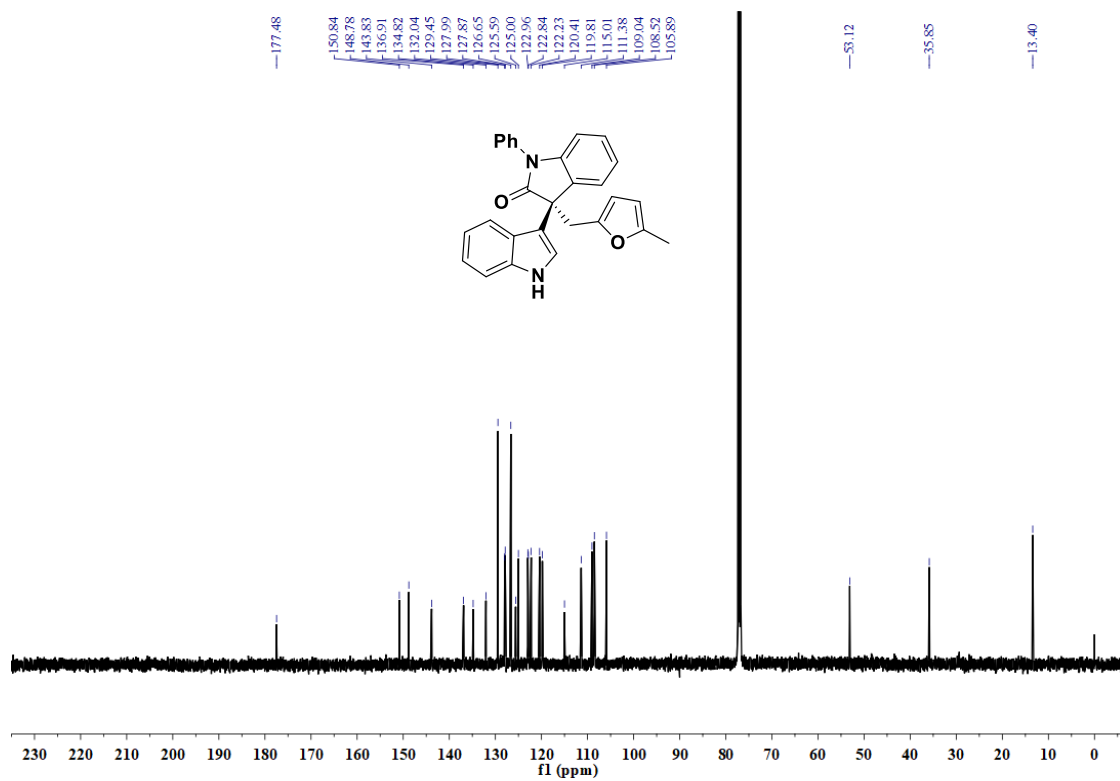
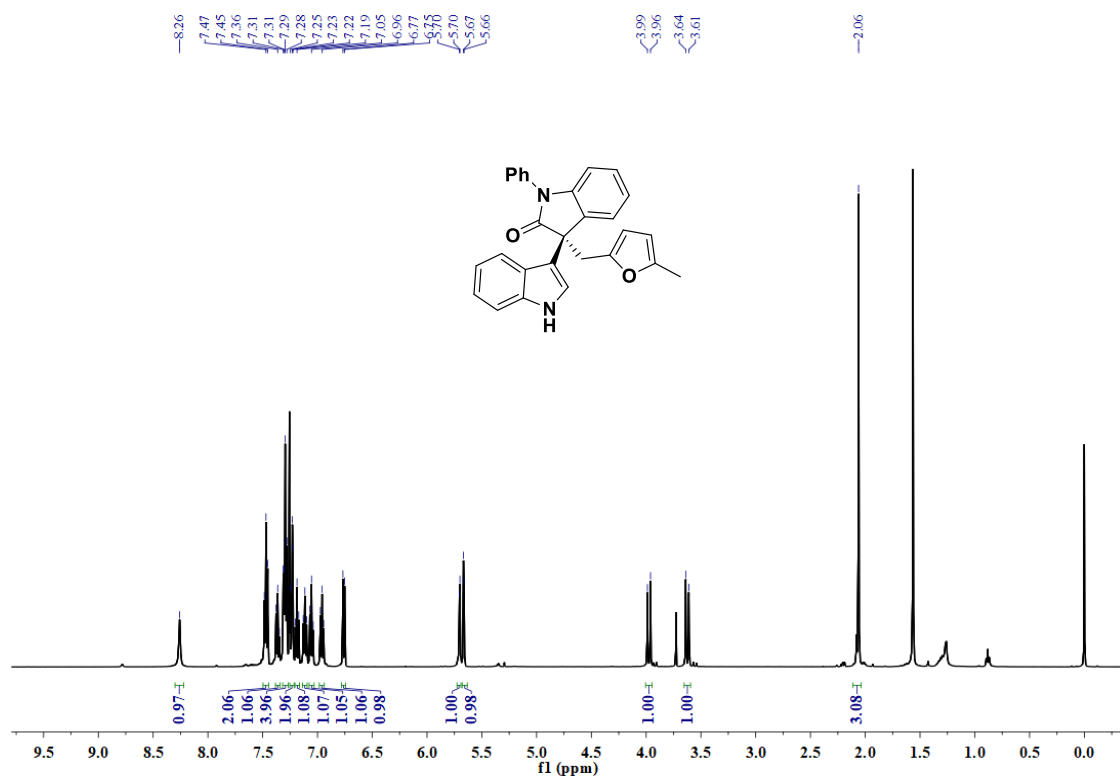
(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-1-propylindolin-2-one(3j)



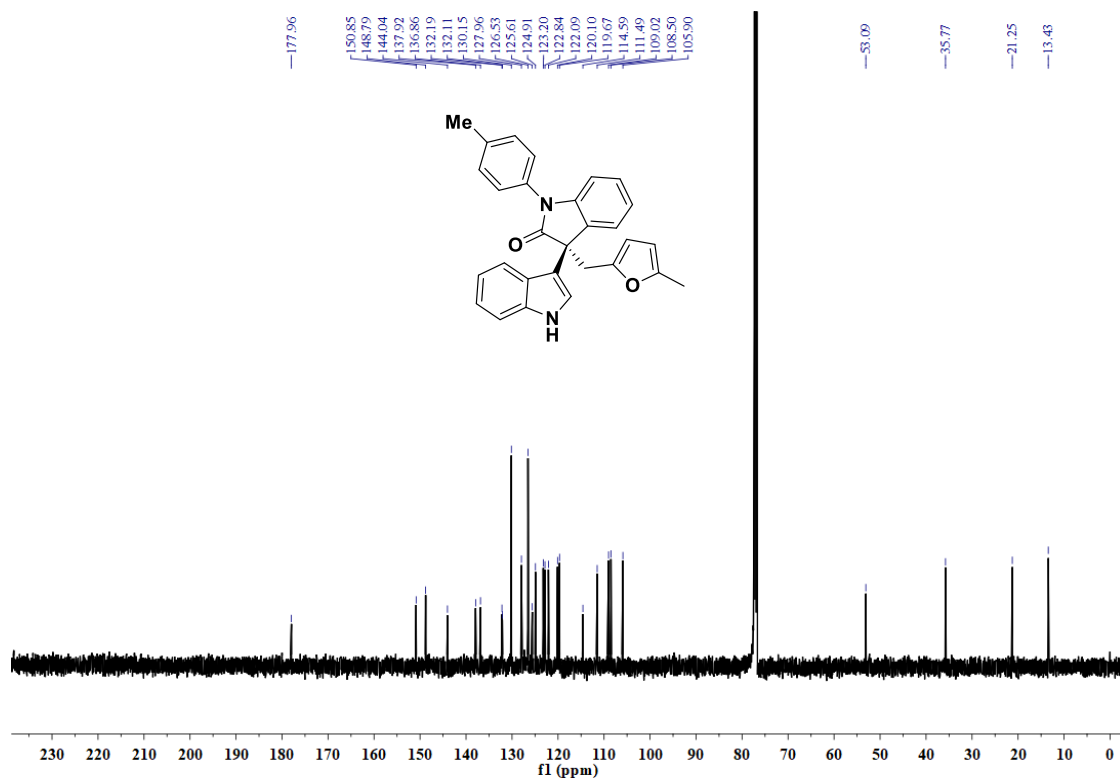
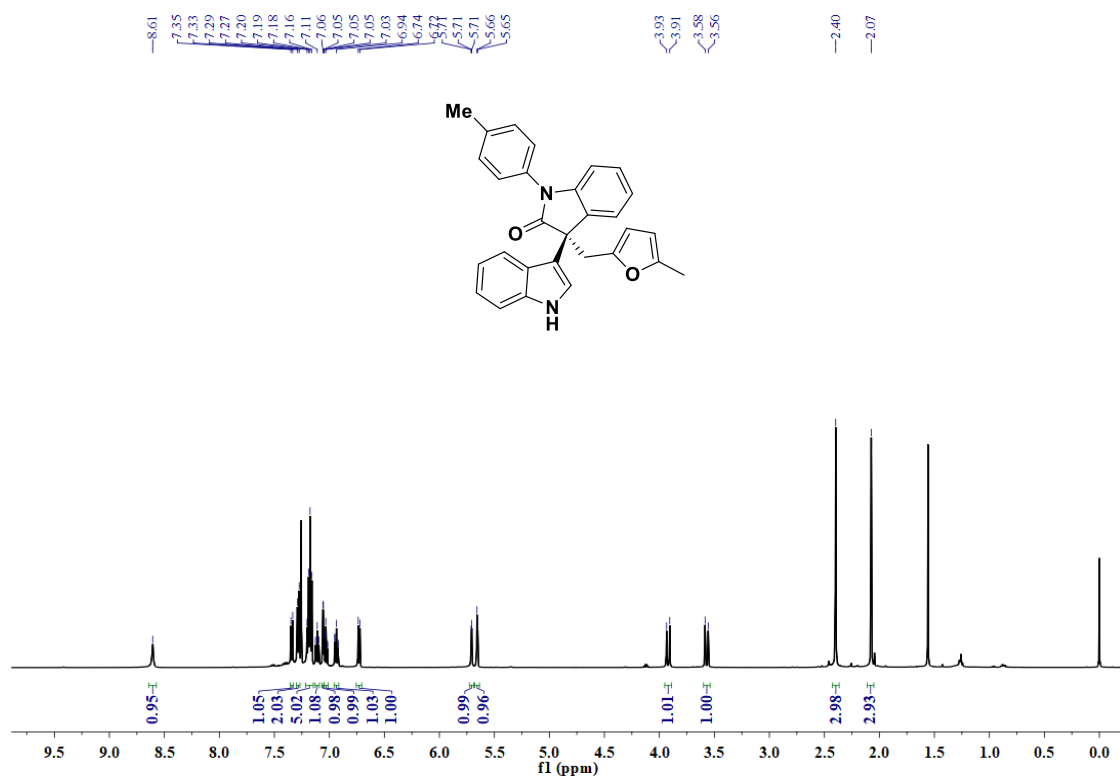
(R)-benzyl-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-2-oxindoline-1-carboxylate(3k)



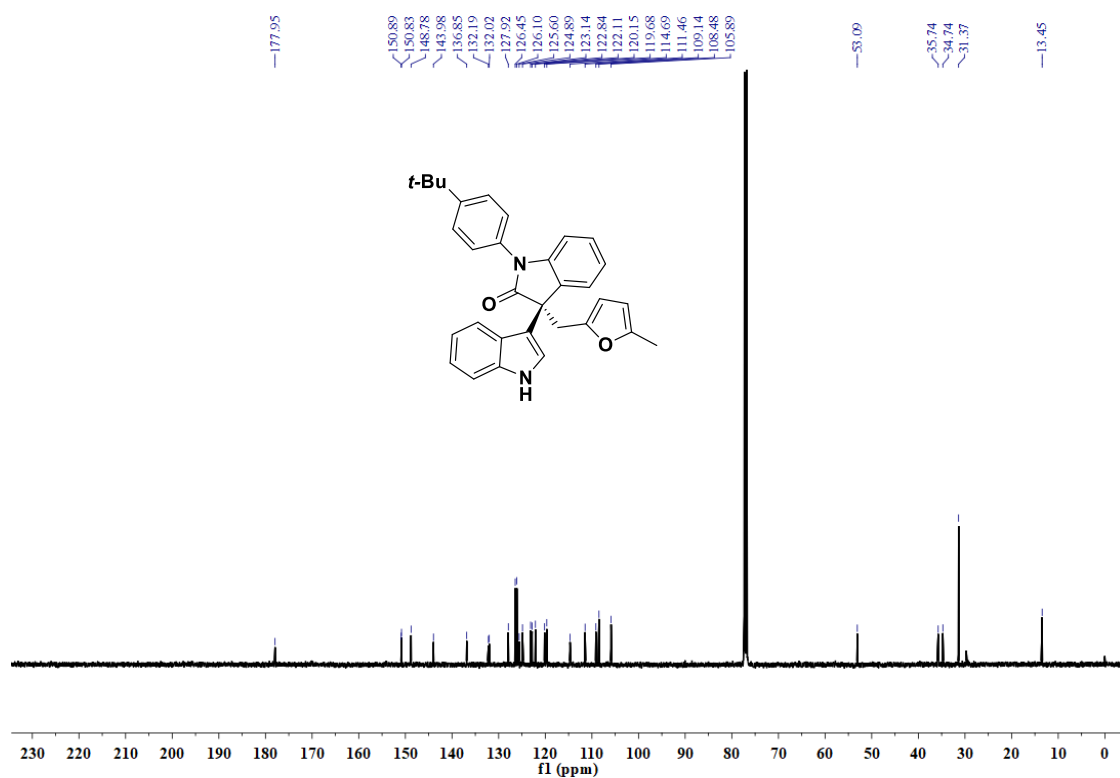
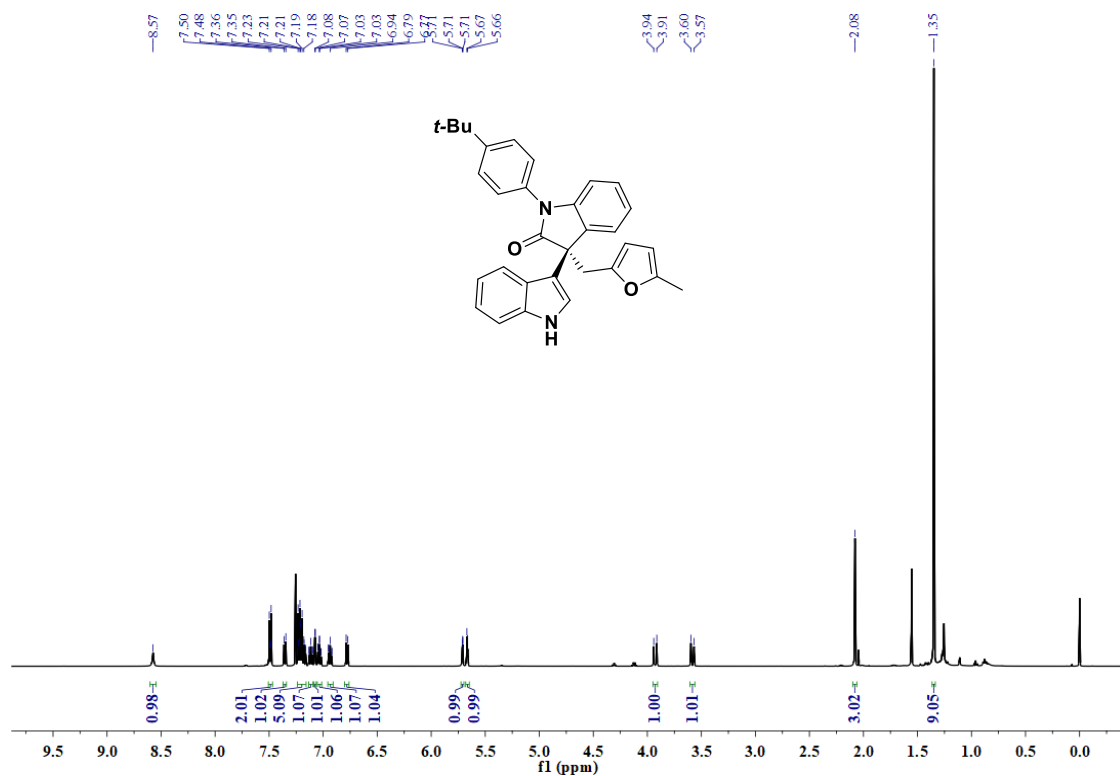
(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-1-phenylindolin-2-one(3l)



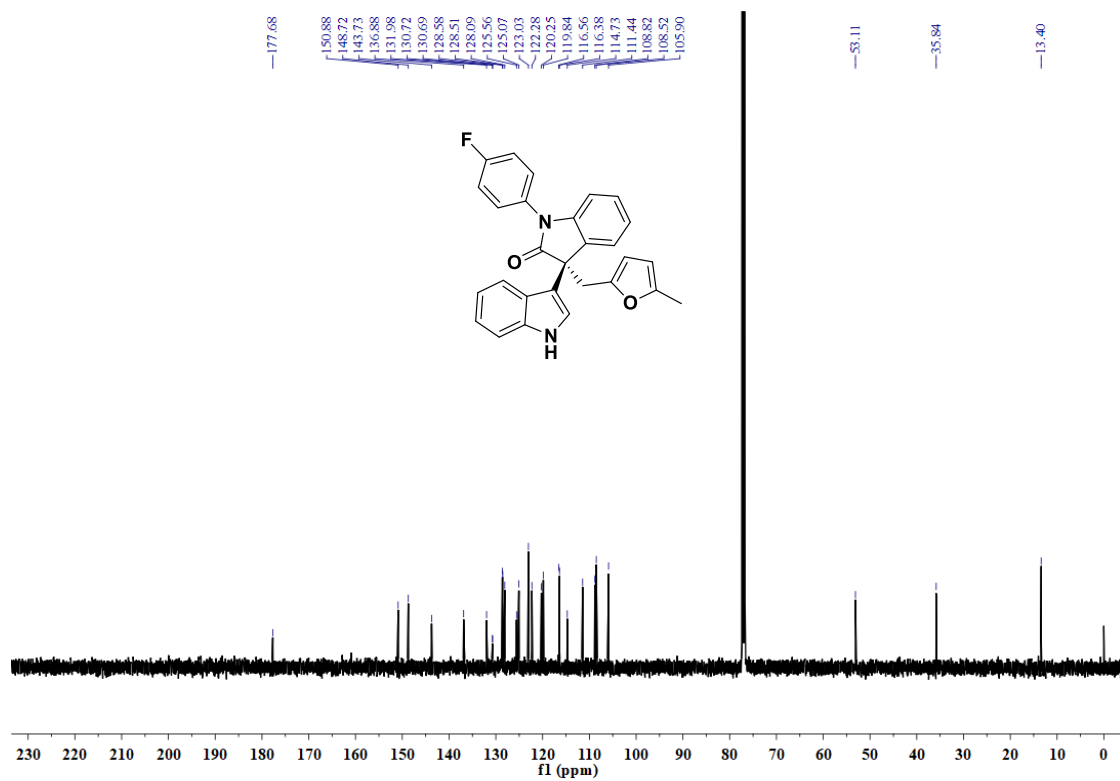
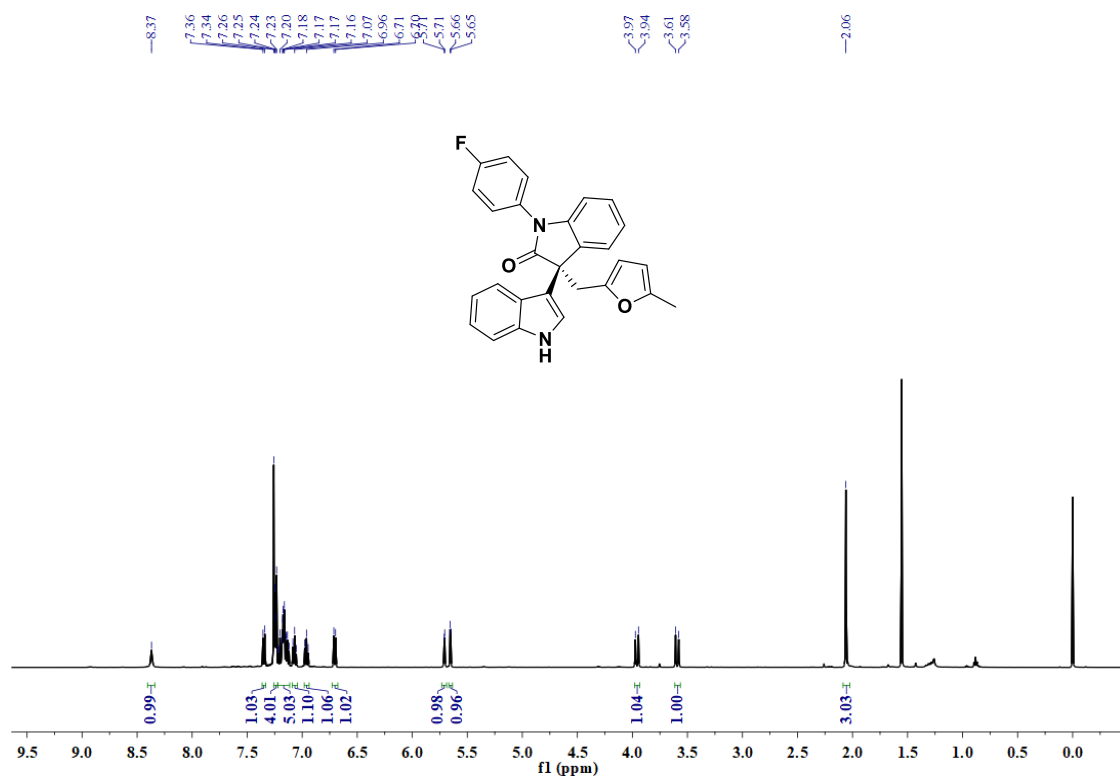
(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)-1-(p-tolyl)indolin-2-one(3m)



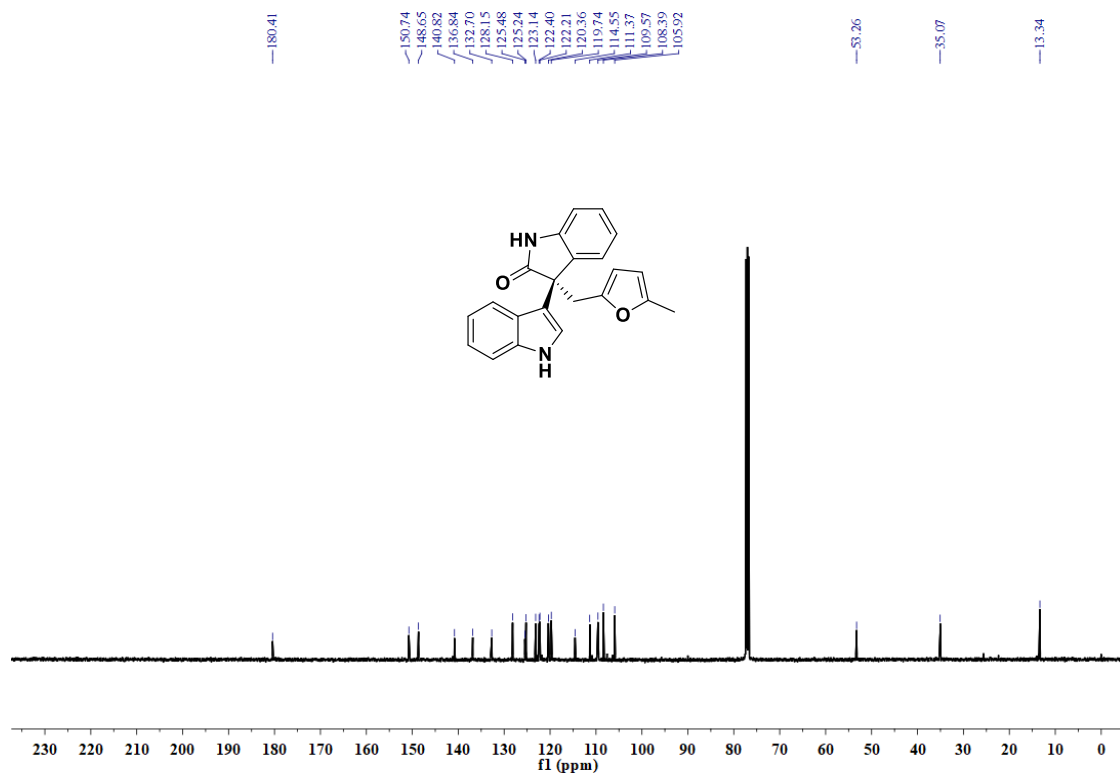
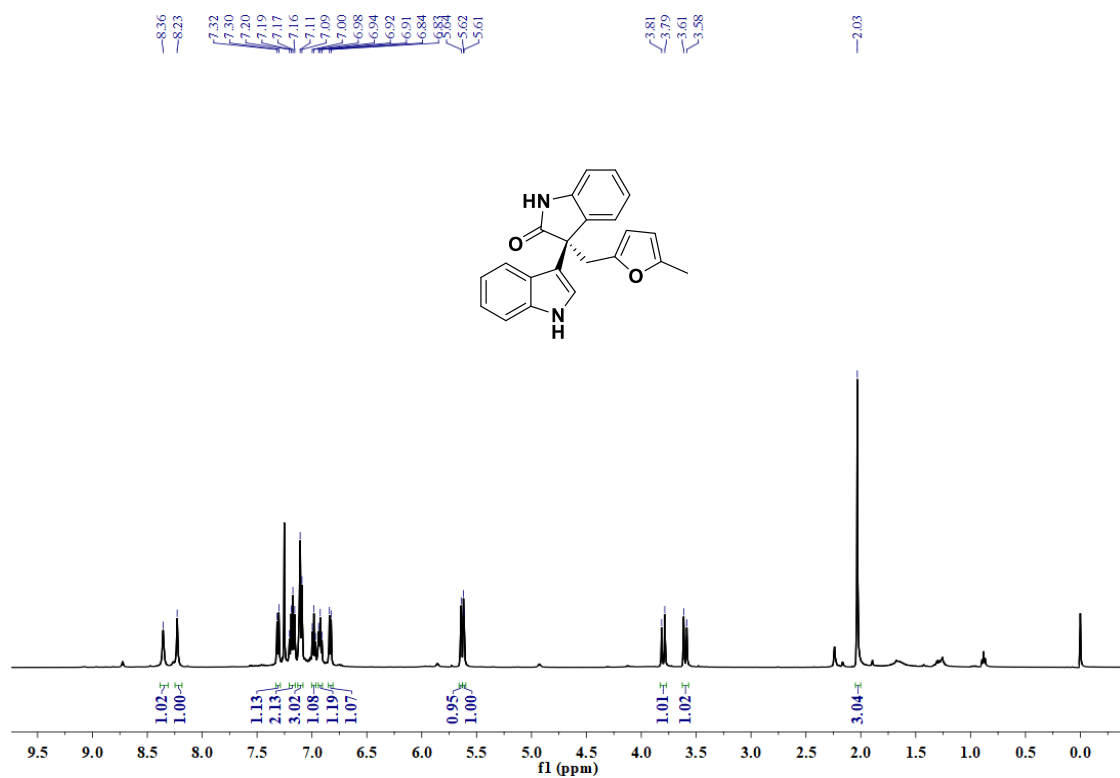
(R)-1-(4-(tert-butyl)phenyl)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3n)



(R)-1-(4-fluorophenyl)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3o)



(R)-3-(1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(3p)



1-benzyl-3-(1-benzyl-5-chloro-1H-indol-3-yl)-3-((5-methylfuran-2-yl)methyl)indolin-2-one(4)

