Supporting Information

Facile, Mild and Highly Enantioselective Alkynylzinc Addition to Aromatic Aldehydes by BINOL/*N*-Methylimidazole Dual Catalysis

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I. General Remarks

NMR spectra were recorded at 300 or 400 MHz (^1H) and at 75 or 100 MHz (^{13}C). The ^1H chemical shifts were measured relative to tetramethylsilane as the internal reference, while the ^{13}C NMR chemical shifts were given using CDCl_3 as the internal standard. Low-resolution mass spectra (MS) were obtained by GC-MS (EI).

All liquid reagents were distilled before use, while the others were used without further purification. $\text{Ti}(\text{O}i\text{Pr})_4$ was distilled under reduced pressure prior to use. Solvents were dried by heating at reflux for at least 24 h over CaH_2 (dichloromethane), or sodium/benzophenone (tetrahydrofuran, toluene and ether) and freshly distilled prior to use. NMI was refluxed with sodium under nitrogen and distilled under reduced pressure. Except as noted, commercial reagents were used as received without further purification. Unless otherwise indicated, all reactions were carried out under dry N_2 atmosphere.

II. General procedure for the preparation of racemic propargylic alcohol

Under argon, *n*-BuLi (0.12 mL, 2.5 M in hexane) was added into a solution of an alkyne (0.35 mmol) in 3 mL of THF at $-78\text{ }^\circ\text{C}$. After the mixture was stirred for 1 h at the same temperature, an aldehyde (0.25 mmol) was then added and the reaction was stirred for additional 3 h. The reaction was then quenched with ice, and the resulting mixture was extracted with CH_2Cl_2 , and the combined organic layers were dried over Mg_2SO_4 . After removal of solvent, the residue was passed through a short silica gel to afford the desired racemic product.

III. General procedure for the catalytic enantioselective addition of alkyne to aldehyde

Under nitrogen, to a flame-dried test tube containing (*R*)-BINOL (7.2 mg, 0.025 mmol) and 3 mL of CH₂Cl₂ were sequentially added NMI (0.0125 mmol, 1 μL), alkyne (0.5 mmol) and Et₂Zn (0.5 mmol, 1.25 M in toluene). The resulting mixture was stirred at room temperature for 2 h, followed by the addition of Ti(OiPr)₄ (0.0625 mmol, 18.5 μL). After one hour of stirring an aldehyde (0.25 mmol) was added, and the resulting mixture was stirred for additional 12 h. Saturated NH₄Cl solution (5 mL) was added to quench the reaction, and the mixture was extracted with ethyl acetate. The combined organic layers were dried over anhydrous MgSO₄ and solvents were removed under reduced pressure. The residue was purified by flash column chromatography (silica gel, 10 % EtOAc in petroleum ether) to give the product.

The yields of asymmetric alkynylation reactions reported are isolated yields and are the averages of two runs at least. The propargylic alcohols are known and their ¹H and ¹³C NMR spectra agreed with those in the literature cited below.¹⁻⁶ The enantiomeric excess (ee) of the products was determined by HPLC using Chiracel OD-H or AD-H column. The absolute configuration of adducts was assigned by comparison to literature data.¹⁻⁷

(S)-1,3-Diphenyl-prop-2-yn-1-ol (3a):¹ 92% yield and 93% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 17.1$ min and $t_{\text{minor}} = 11.8$ min; ¹H NMR (300 MHz, CDCl₃) δ 2.56 (br, 1H), 5.70 (s, 1H), 7.30-7.50 (m, 8H), 7.62-7.65 (m, 2H); GC-MS: m/z 208 [M⁺].

Rank	Time	Quantity	Area	Height
1	11.793	3.371	376210	14957
2	17.057	96.63	10782157	287803
Total		100	11158367	302760

(S)-1-(2-Methylphenyl)-3-phenyl-prop-2-yn-1-ol (3b):¹ 91% yield and 93% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 17.8$ min and $t_{\text{minor}} = 10.3$ min; ¹H NMR (300 MHz, CDCl₃) δ 2.04 (br, 1H), 2.38 (s, 3H), 5.72 (s, 1H), 7.06-7.20 (m, 6H), 7.32-7.35 (m, 2H), 7.59-7.62 (m, 1H); GC-MS: m/z 223 [M+1]⁺.

Rank	Time	Quantity	Area	Height
1	10.347	3.564	194284	10135
2	17.803	96.43	5256212	139622
Total		100	5450496	149757

(S)-1-(3-Methylphenyl)-3-phenyl-prop-2-yn-1-ol (3c):¹ 92% yield and 94% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 22.5$ min and $t_{\text{minor}} = 10.9$ min; ¹H NMR (300 MHz, CDCl₃) δ 2.23 (br, 1H), 2.32 (s, 3H), 5.58 (s, 1H), 7.08 (d, $J = 7.5$ Hz, 1H), 7.18-7.27 (m, 4H), 7.33-7.43 (m, 4H); GC-MS: m/z 222[M⁺].

Rank	Time	Quantity	Area	Height
1	10.893	3.224	108769	4849
2	22.507	96.77	3264367	62315
Total		100	3373136	67164

(S)-1-(4-Methylphenyl)-3-phenyl-prop-2-yn-1-ol (3d):² 81% yield and 92% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 17.1$ min and $t_{\text{minor}} = 9.2$ min; ¹H NMR (300 MHz, CDCl₃) δ 2.20 (br, 1H), 2.29 (s, 3H), 5.58 (s, 1H), 7.12-7.15 (d, $J = 7.8$ Hz, 2H), 7.22-7.27 (m, 3H), 7.37-7.44 (m, 4H); GC-MS: m/z 222 [M⁺].

Rank	Time	Quantity	Area	Height
1	9.200	4.144	153082	7926
2	17.097	95.85	3540723	91607
Total		100	3693805	99533

(S)-1-(3-Chlorophenyl)-3-phenyl-prop-2-yn-1-ol (3e):¹ 95% yield and 92% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 25.5$ min and $t_{\text{minor}} = 8.5$ min; ¹H NMR (400 MHz, CDCl₃) δ 2.47 (br, 1H), 5.66 (s, 1H), 7.30-7.35 (m, 5H), 7.46-7.50 (m, 3H), 7.61 (s, 1H); GC-MS: m/z 241 [M-1]⁺.

Rank	Time	Quantity	Area	Height
1	8.473	3.887	180615	10141
2	25.533	96.12	4466738	79117
Total		100	4647353	89258

(S)-1-(4-Chlorophenyl)-3-phenyl-prop-2-yn-1-ol (3f):¹ 80% yield and 92% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 21.3$ min and $t_{\text{minor}} = 9.8$ min; ¹H NMR (300 MHz, CDCl₃) δ 2.38 (br, 1H), 5.67(s, 1H), 7.32-7.40 (m, 5H), 7.45-7.50 (m, 2H), 7.53-7.57 (m, 2H); GC-MS: m/z 241 [M-1]⁺.

Rank	Time	Quantity	Area	Height
1	9.793	4.075	150382	8614
2	21.277	95.92	3540240	92272
Total		100	3690622	100886

(S)-1-(4-Bromophenyl)-3-phenyl-prop-2-yn-1-ol (3g):² 85% yield and 92% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 24.8$ min and $t_{\text{minor}} = 9.3$ min; ^1H NMR (400 MHz, CDCl_3) δ 2.37 (br, 1H), 5.66 (s, 1H), 7.31-7.35 (m, 3H), 7.46-7.55 (m, 6H); GC-MS: m/z 286 $[\text{M}^+]$.

Rank	Time	Quantity	Area	Height
1	9.333	4.258	366129	19683
2	24.837	95.74	8232117	154766
Total		100	8598246	174449

(S)-1-(4-Fluorophenyl)-3-phenyl-prop-2-yn-1-ol (3h):¹ 91% yield and 93% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 19.6$ min and $t_{\text{minor}} = 8.4$ min; ^1H NMR (300 MHz, CDCl_3) δ 2.58 (br, 1H), 5.67 (s, 1H), 7.04-7.12 (m, 2H), 7.29-7.37 (m, 3H), 7.45-7.50 (m, 2H), 7.56-7.62 (m, 2H); GC-MS: m/z 225 $[\text{M}-1]^+$.

Rank	Time	Quantity	Area	Height
1	8.360	3.466	202695	12496
2	19.633	96.54	5644804	140933
Total	100	5847499	153429

(S)-1-(4-Methoxyphenyl)-3-phenyl-prop-2-yn-1-ol (3i):² 87% yield and 93% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 25.2$ min and $t_{\text{minor}} = 14.8$ min; ^1H NMR (300 MHz, CDCl_3) δ 2.17 (br, 1H), 3.75 (s, 3H), 5.58 (s, 1H), 6.85-6.88 (m, 2H), 7.24-7.26 (m, 3H), 7.39-7.42 (m, 2H), 7.46-7.49 (m, 2H); GC-MS: m/z 238 [M^+].

Rank	Time	Quantity	Area	Height
1	14.750	3.765	104084	3189
2	25.243	96.23	2660612	43420
Total		100	2764696	46609

(S)-1-(3-Methoxyphenyl)-3-phenylprop-2-yn-1-ol (3j):¹ 82% yield and 91% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 24.0$ min and $t_{\text{minor}} = 17.8$ min; ¹H NMR (400 MHz, CDCl₃) δ 2.48 (br, 1H), 3.82 (s, 3H), 5.66 (s, 1H), 6.87-6.90 (m, 1H), 7.17-7.20 (m, 2H), 7.28-7.33 (m, 4H), 7.45-7.48 (m, 2H); GC-MS: m/z 238 [M⁺].

Rank	Time	Quantity	Area	Height
1	17.827	4.353	1196006	25916
2	24.047	95.64	26278520	384172
Total		100	27474526	410088

(S)-1-(2-Furyl)-3-phenylprop-2-yn-1-ol (3k):² 92% yield and 87% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 18.0$ min and $t_{\text{minor}} = 9.2$ min; ¹H NMR (300 MHz, CDCl₃) δ 2.40 (br, 1H), 5.62 (s, 1H), 6.30 (2d, $J = 2.0, 1.6$ Hz, 1H), 6.45 (d, $J = 3.0$ Hz, 1H), 7.21-7.27 (m, 3H), 7.37-7.43 (m, 3H); GC-MS: m/z 197 [M-1]⁺.

Rank	Time	Quantity	Area	Height
1	9.203	6.673	316620	15390
2	18.017	93.32	4428144	106297
Total		100	4744764	121687

(S)-1-(2-Naphthyl)-3-phenyl-prop-2-yn-1-ol (3l):¹ 85% yield and 93% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 40.5$ min and $t_{\text{minor}} = 13.5$ min; ¹H NMR (400 MHz, CDCl₃) δ 2.40 (br, 1H), 5.87 (s, 1H), 7.31-7.36 (m, 3H), 7.48-7.54 (m, 4H), 7.73 (2d, $J = 2.0, 1.6$ Hz, 1H), 7.84-7.91 (m, 3H), 8.07 (s, 1H); GC-MS: m/z 258 [M⁺].

Rank	Time	Quantity	Area	Height
1	13.493	3.734	271959	8834
2	40.540	96.26	7010101	70741
Total		100	7282059	79575

(S)-Methyl 4-hydroxy-4-phenylbut-2-ynoate (3m):³ 68% yield and 88% ee determined by HPLC analysis (Chiralcel OD-H column, 10% *i*PrOH in hexane at 1.0 mL/min, 254 nm); Retention time: $t_{\text{major}} = 11.6$ min and $t_{\text{minor}} = 15.9$ min; ^1H NMR (400 MHz, CDCl_3) δ 2.61 (br, 1H), 3.78 (s, 3H), 5.56 (s, 1H), 7.34-7.42 (m, 3H), 7.50-7.52 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ 52.9, 64.2, 77.5, 86.6, 126.6, 128.8, 128.9, 138.5, 153.8; GC-MS: m/z 190 $[\text{M}^+]$.

Rank	Time	Quantity	Area	Height
1	11.643	94	16043269	511288
2	15.863	5.994	1022938	24011
Total		100	17066207	535299

(S)-1-Phenyl-3-(1-cyclohexenyl)-prop-2-yn-1-ol (3n):⁴ 91% yield and 89% ee determined by HPLC analysis (Chiralcel OD-H column, 5% *i*PrOH in hexane at 1.0 mL/min, 254 nm). Retention time: $t_{\text{major}} = 10.2$ min and $t_{\text{minor}} = 16.5$ min; ^1H NMR (400 MHz, CDCl_3) δ 1.55-1.67 (m, 4H), 2.09-2.17 (m, 4H), 2.20 (br, 1H), 5.57 (s, 1H), 6.16-6.18 (m, 1H), 7.30-7.40 (m, 3H), 7.55-7.57 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ 21.4, 22.2, 25.6, 29.1, 65.1, 86.7, 88.6, 120.6, 126.7, 128.2, 128.6, 135.7; GC-MS: m/z 211 $[\text{M}-1]^+$.

Rank	Time	Quantity	Area	Height
1	10.203	94.35	4804131	181220
2	16.497	5.65	287679	7546
Total		100	5091810	188766

(S)-1-Phenyl-3-cyclopropyl-prop-2-yn-1-ol (3o):⁵ 78% yield and 88% ee determined by HPLC analysis (Chiralcel OD-H column, 5% *i*PrOH in hexane at 1.0 mL/min, 214 nm); Retention time: $t_{\text{major}} = 10.9$ min and $t_{\text{minor}} = 19.4$ min; ^1H NMR (400 MHz, CDCl_3) δ 0.69-0.80 (m, 4H), 1.26-1.33 (m, 1H), 2.47 (br, 1H), 5.38 (s, 1H), 7.27-7.37 (m, 3H), 7.48-7.51 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ -0.4, 8.3, 64.7, 75.2, 90.6, 126.6, 128.2, 128.5, 141.2; GC-MS: m/z 172 [M^+].

Rank	Time	Quantity	Area	Height
1	10.887	93.79	14742986	499287
2	19.373	6.21	976160	22073
Total		100	15719146	521360

(S)-1-Phenyl-3-trimethylsilyl-prop-2-yn-1-ol (3p):^{6, 7} 88% yield and 91% ee determined by HPLC analysis (Chiralcel OD-H column, 5% *i*PrOH in hexane at 1.0 mL/min, 214 nm); Retention time: $t_{\text{major}} = 5.3$ min and $t_{\text{minor}} = 9.5$ min; ^1H NMR (300 MHz, CDCl_3) δ 0.21 (s, 9H), 2.07 (br, 1H), 5.45 (s, 1H), 7.31-7.41 (m, 3H), 7.53-7.56 (m, 2H). ^{13}C NMR (100 MHz, CDCl_3) δ -0.2, 65.0, 91.6, 104.9, 126.7, 128.4, 128.5, 140.3; GC-MS: m/z 204 [M^+].

Rank	Time	Quantity	Area	Height
1	5.347	95.65	5489606	470660
2	9.493	4.351	249705	11949
Total		100	5739312	482609

(S)-1-(3-Methoxyphenyl)-3-trimethylsilyl-prop-2-yn-1-ol (3q):⁶ 82% yield and 93% ee determined by HPLC analysis (Chiralcel AD-H column, 2% *i*PrOH in hexane at 1.0 mL/min, 214 nm); Retention time: $t_{\text{major}} = 12.6$ min and $t_{\text{minor}} = 15.9$ min; ^1H NMR (400 MHz, CDCl_3) δ 0.20 (s, 9H), 2.38 (br, 1H), 3.80 (s, 3H), 5.42 (s, 1H), 6.85-6.88 (m, 1H), 7.10-7.12 (m, 2H), 7.25-7.31 (m, 1H).; ^{13}C NMR (100 MHz, CDCl_3) δ -0.2, 55.2, 64.8, 91.5, 104.9, 112.0, 114.1, 119.0, 130.0, 141.9, 159.7; GC-MS: m/z 234 [M^+].

Rank	Time	Quantity	Area	Height
1	12.603	96.33	17887829	724605
2	15.857	3.669	681265	16804
Total		100	18569093	741409

(S)-1-(4-Fluorophenyl)-3-trimethylsilyl-prop-2-yn-1-ol (3r):⁶ 80% yield and 93% ee determined by HPLC analysis (Chiralcel AD-H column, 2% *i*PrOH in hexane at 1.0 mL/min, 214 nm); Retention time: $t_{\text{major}} = 8.1$ min and $t_{\text{minor}} = 9.4$ min; ^1H NMR (400 MHz, CDCl_3) δ 0.21 (s, 9H), 2.37 (br, 1H), 5.43 (s, 1H), 7.03-7.09 (m, 2H), 7.49-7.53 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ -0.3, 64.2, 91.8, 104.7, 115.2 (d, $J_{\text{C,F}} = 21.6$ Hz), 128.5 (d, $J_{\text{C,F}} = 8.4$ Hz), 136.1, 161.4 (d, $J_{\text{C,F}} = 246.0$ Hz); GC-MS: m/z 222 [M^+].

Rank	Time	Quantity	Area	Height
1	8.140	96.59	10455702	713618
2	9.353	3.408	368875	21779
Total	100	10824577	735397	

IV. References:

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- (4) Li, Z. B.; Pu, L. *Org. Lett.* **2004**, *6*, 1065.
- (5) Jiang, B.; Feng, Y. *Tetrahedron Lett.* **2002**, *43*, 2975.
- (6) Wolf, C.; Liu, S. L. *J. Am. Chem. Soc.* **2006**, *128*, 10996.
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V. Copies of ^1H and ^{13}C NMR spectra for compounds 3a-3r:

Chemical structure of 3e: c1ccccc1C#CC(O)c2ccc(Cl)cc2

¹H NMR spectrum (CDCl₃):

- Chemical shift range: 10 to 0 ppm.
- Peak list (ppm): 7.613, 7.501, 7.497, 7.483, 7.479, 7.465, 7.460, 7.352, 7.348, 7.338, 7.335, 7.312, 7.316, 7.307, 7.297, 7.252, 5.664, 2.471, 1.591, 1.589, 1.587, 1.585, 1.583, 1.581, 1.579, 1.577, 1.575, 1.573, 1.571, 1.569, 1.567, 1.565, 1.563, 1.561, 1.559, 1.557, 1.555, 1.553, 1.551, 1.549, 1.547, 1.545, 1.543, 1.541, 1.539, 1.537, 1.535, 1.533, 1.531, 1.529, 1.527, 1.525, 1.523, 1.521, 1.519, 1.517, 1.515, 1.513, 1.511, 1.509, 1.507, 1.505, 1.503, 1.501, 1.499, 1.497, 1.495, 1.493, 1.491, 1.489, 1.487, 1.485, 1.483, 1.481, 1.479, 1.477, 1.475, 1.473, 1.471, 1.469, 1.467, 1.465, 1.463, 1.461, 1.459, 1.457, 1.455, 1.453, 1.451, 1.449, 1.447, 1.445, 1.443, 1.441, 1.439, 1.437, 1.435, 1.433, 1.431, 1.429, 1.427, 1.425, 1.423, 1.421, 1.419, 1.417, 1.415, 1.413, 1.411, 1.409, 1.407, 1.405, 1.403, 1.401, 1.399, 1.397, 1.395, 1.393, 1.391, 1.389, 1.387, 1.385, 1.383, 1.381, 1.379, 1.377, 1.375, 1.373, 1.371, 1.369, 1.367, 1.365, 1.363, 1.361, 1.359, 1.357, 1.355, 1.353, 1.351, 1.349, 1.347, 1.345, 1.343, 1.341, 1.339, 1.337, 1.335, 1.333, 1.331, 1.329, 1.327, 1.325, 1.323, 1.321, 1.319, 1.317, 1.315, 1.313, 1.311, 1.309, 1.307, 1.305, 1.303, 1.301, 1.299, 1.297, 1.295, 1.293, 1.291, 1.289, 1.287, 1.285, 1.283, 1.281, 1.279, 1.277, 1.275, 1.273, 1.271, 1.269, 1.267, 1.265, 1.263, 1.261, 1.259, 1.257, 1.255, 1.253, 1.251, 1.249, 1.247, 1.245, 1.243, 1.241, 1.239, 1.237, 1.235, 1.233, 1.231, 1.229, 1.227, 1.225, 1.223, 1.221, 1.219, 1.217, 1.215, 1.213, 1.211, 1.209, 1.207, 1.205, 1.203, 1.201, 1.199, 1.197, 1.195, 1.193, 1.191, 1.189, 1.187, 1.185, 1.183, 1.181, 1.179, 1.177, 1.175, 1.173, 1.171, 1.169, 1.167, 1.165, 1.163, 1.161, 1.159, 1.157, 1.155, 1.153, 1.151, 1.149, 1.147, 1.145, 1.143, 1.141, 1.139, 1.137, 1.135, 1.133, 1.131, 1.129, 1.127, 1.125, 1.123, 1.121, 1.119, 1.117, 1.115, 1.113, 1.111, 1.109, 1.107, 1.105, 1.103, 1.101, 1.099, 1.097, 1.095, 1.093, 1.091, 1.089, 1.087, 1.085, 1.083, 1.081, 1.079, 1.077, 1.075, 1.073, 1.071, 1.069, 1.067, 1.065, 1.063, 1.061, 1.059, 1.057, 1.055, 1.053, 1.051, 1.049, 1.047, 1.045, 1.043, 1.041, 1.039, 1.037, 1.035, 1.033, 1.031, 1.029, 1.027, 1.025, 1.023, 1.021, 1.019, 1.017, 1.015, 1.013, 1.011, 1.009, 1.007, 1.005, 1.003, 1.001, 0.999, 0.997, 0.995, 0.993, 0.991, 0.989, 0.987, 0.985, 0.983, 0.981, 0.979, 0.977, 0.975, 0.973, 0.971, 0.969, 0.967, 0.965, 0.963, 0.961, 0.959, 0.957, 0.955, 0.953, 0.951, 0.949, 0.947, 0.945, 0.943, 0.941, 0.939, 0.937, 0.935, 0.933, 0.931, 0.929, 0.927, 0.925, 0.923, 0.921, 0.919, 0.917, 0.915, 0.913, 0.911, 0.909, 0.907, 0.905, 0.903, 0.901, 0.899, 0.897, 0.895, 0.893, 0.891, 0.889, 0.887, 0.885, 0.883, 0.881, 0.879, 0.877, 0.875, 0.873, 0.871, 0.869, 0.867, 0.865, 0.863, 0.861, 0.859, 0.857, 0.855, 0.853, 0.851, 0.849, 0.847, 0.845, 0.843, 0.841, 0.839, 0.837, 0.835, 0.833, 0.831, 0.829, 0.827, 0.825, 0.823, 0.821, 0.819, 0.817, 0.815, 0.813, 0.811, 0.809, 0.807, 0.805, 0.803, 0.801, 0.799, 0.797, 0.795, 0.793, 0.791, 0.789, 0.787, 0.785, 0.783, 0.781, 0.779, 0.777, 0.775, 0.773, 0.771, 0.769, 0.767, 0.765, 0.763, 0.761, 0.759, 0.757, 0.755, 0.753, 0.751, 0.749, 0.747, 0.745, 0.743, 0.741, 0.739, 0.737, 0.735, 0.733, 0.731, 0.729, 0.727, 0.725, 0.723, 0.721, 0.719, 0.717, 0.715, 0.713, 0.711, 0.709, 0.707, 0.705, 0.703, 0.701, 0.699, 0.697, 0.695, 0.693, 0.691, 0.689, 0.687, 0.685, 0.683, 0.681, 0.679, 0.677, 0.675, 0.673, 0.671, 0.669, 0.667, 0.665, 0.663, 0.661, 0.659, 0.657, 0.655, 0.653, 0.651, 0.649, 0.647, 0.645, 0.643, 0.641, 0.639, 0.637, 0.635, 0.633, 0.631, 0.629, 0.627, 0.625, 0.623, 0.621, 0.619, 0.617, 0.615, 0.613, 0.611, 0.609, 0.607, 0.605, 0.603, 0.601, 0.599, 0.597, 0.595, 0.593, 0.591, 0.589, 0.587, 0.585, 0.583, 0.581, 0.579, 0.577, 0.575, 0.573, 0.571, 0.569, 0.567, 0.565, 0.563, 0.561, 0.559, 0.557, 0.555, 0.553, 0.551, 0.549, 0.547, 0.545, 0.543, 0.541, 0.539, 0.537, 0.535, 0.533, 0.531, 0.529, 0.527, 0.525, 0.523, 0.521, 0.519, 0.517, 0.515, 0

RA-15 H1 CDC13 2006-3-24
Pulse Sequence: s2pu1

Ra-3

Current Data Parameters
NAME Ra-3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060307
Time 16.35
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 8
DS 4
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 90.5
DW 83.400 usec
DE 6.00 usec
TE 294.1 K
D1 2.50000000 sec
TD0 1

CHANNEL f1
NUC1 1H
P1 7.70 usec
PL1 -5.00 dB
SFO1 300.1324010 MHz

F2 - Processing parameters
SI 16384
SF 300.1300066 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RA1-41 H1 CDC13 2007-1-25
Pulse Sequence: s2pu1

Ra-9

Current Data Parameters
NAME Ra-9
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20060313
Time 16.49
INSTRUM av300
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 32768
SOLVENT CDCl3
NS 16
DS 4
SWH 5995.204 Hz
FIDRES 0.182959 Hz
AQ 2.7329011 sec
RG 181
DW 83.400 usec
DE 6.00 usec
TE 293.6 K
D1 2.5000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 7.70 usec
PL1 -5.00 dB
SFO1 300.1324010 MHz

F2 - Processing parameters
SI 16384
SF 300.1300297 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.40

RA-14 H1, CDC13 2006-3-24
Pulse Sequence: s2pul

Ra1-34 M1 CDC13 2006-12-20
Pulse Sequence: s2pu1

Ra1-34 C13 CDC13 2006-12-22
Pulse Sequence: s2pu1

RA1-39 H1 CDC13 2007-1-18
Pulse Sequence: s2pu1

RA1-39-CDCL3-C13-2007-1-19
Pulse Sequence: s2pu1

RA1-36 H1 CDCl3 2007-1-18
Pulse Sequence: s2pu1

RA1-36-CDCL3-C13-2007-1-19
Pulse Sequence: s2pu1

1-30Ra H1 CDC13 2006-12-11
Pulse Sequence: s2pul

1-30Ra C13 CDC13 2006-12-14
Pulse Sequence: s2pul

RA1-42 H1 CDC13 2007-1-25
Pulse Sequence: s2pu1

Ra1-42-CDCL3-C13-2007-1-27
Pulse Sequence: s2pu1

RA1-43 H1 CDC13 2007-1-25
Pulse Sequence: s2pu1

Ra1-43-CDCL3-C13-2007-1-27
Pulse Sequence: s2pu1