

## Supporting Information for

# Kilo-Scale Buchwald-Hartwig Amination: Optimized Coupling of Base-Sensitive 6-Bromoisoquinoline-1-Carbonitrile with (S)-3-Amino-2-Methylpropan-1-ol

*Jeffrey B. Sperry,<sup>\*,†</sup> Kristin E. Price Wigglesworth,<sup>†</sup> Ian Edmonds,<sup>⊥</sup> Phillip J. Fiore,<sup>⊥</sup> David C. Boyles,<sup>†</sup> David B. Damon,<sup>†</sup> Roberta L. Dorow,<sup>†</sup> Eugene L. Piatnitski Chekler,<sup>‡</sup> Jonathan Langille,<sup>‡</sup> and Jotham W. Coe<sup>‡</sup>*

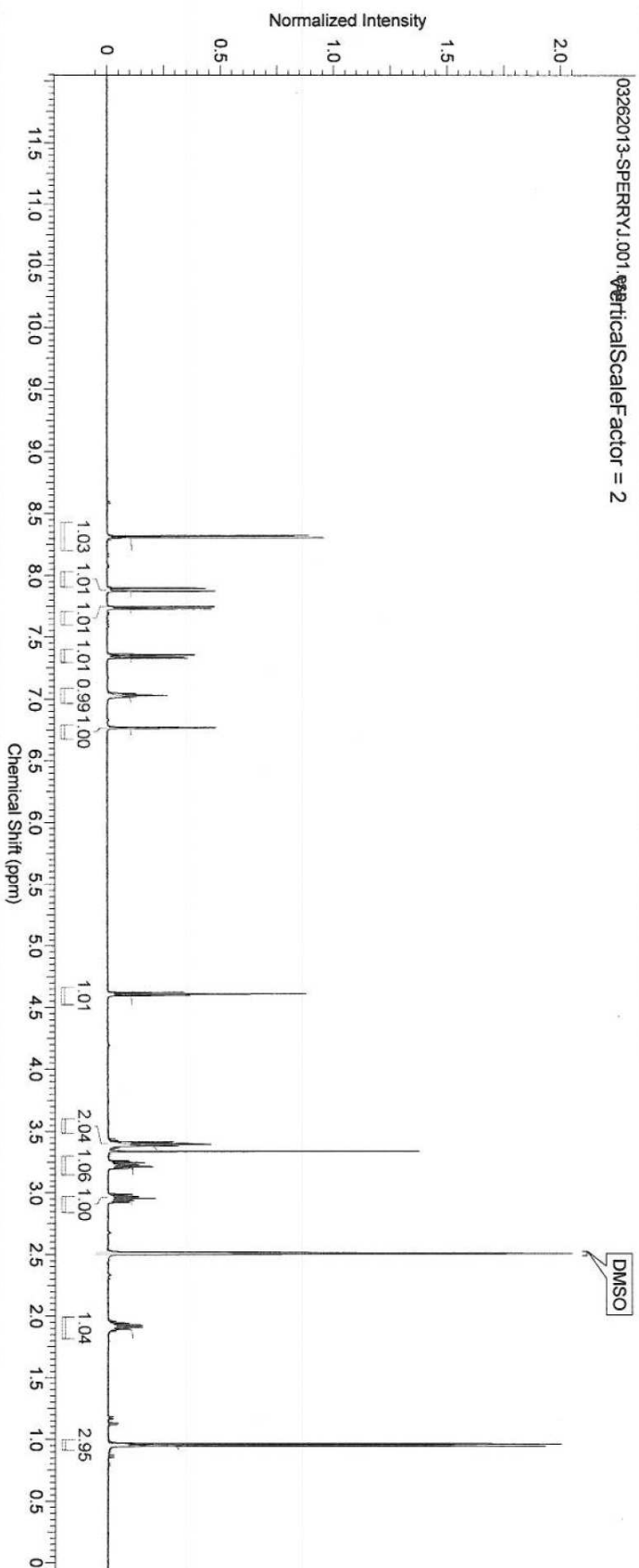
<sup>†</sup>Chemical Research and Development, Pfizer Inc., 558 Eastern Point Rd., Groton, CT 06340

<sup>⊥</sup>Bridge Organics, 311 W. Washington St., Vicksburg, MI, 49097

<sup>‡</sup>Pfizer Worldwide Medicinal Chemistry, Pfizer Inc, 558 Eastern Point Rd., Groton, CT 06340

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| SI-2        | <sup>1</sup> H NMR spectrum of (S)-3 in DMSO- <i>d</i> <sub>6</sub>  |
| SI-3        | <sup>13</sup> C NMR spectrum of (S)-3 in DMSO- <i>d</i> <sub>6</sub> |

|                                |                      |                   |                                                                |                        |                      |
|--------------------------------|----------------------|-------------------|----------------------------------------------------------------|------------------------|----------------------|
| Acquisition Time (sec)         | 3.9846               | Comment           | 705714-021-01 PROTON DMSO (aplttopspin sperry) 22              | Date                   | 26 Mar 2013 13:16:48 |
| Date Stamp                     | 26 Mar 2013 13:16:48 | File Name         | \\SEG7\OADAT\AIBH091709\DAT\ASPERRYJ\NMRO3262013-SPERRYJ\1\FID | Origin                 | spec                 |
| Frequency (MHz)                | 400.13               | Nucleus           | <sup>1</sup> H                                                 | Number of Transients   | 16                   |
| Original Points Count          | 32768                | Owner             | nmr                                                            | Points Count           | 32768                |
| Receiver Gain                  | 203.00               | SW(cyclical) (Hz) | 8223.68                                                        | Solvent                | DMSO-d6              |
| Spectrum Type                  | STANDARD             | Sweep Width (Hz)  | 8223.43                                                        | Temperature (degree C) | 22.300               |
| Spectrum Offset (Hz) 2470.9683 |                      |                   |                                                                |                        |                      |

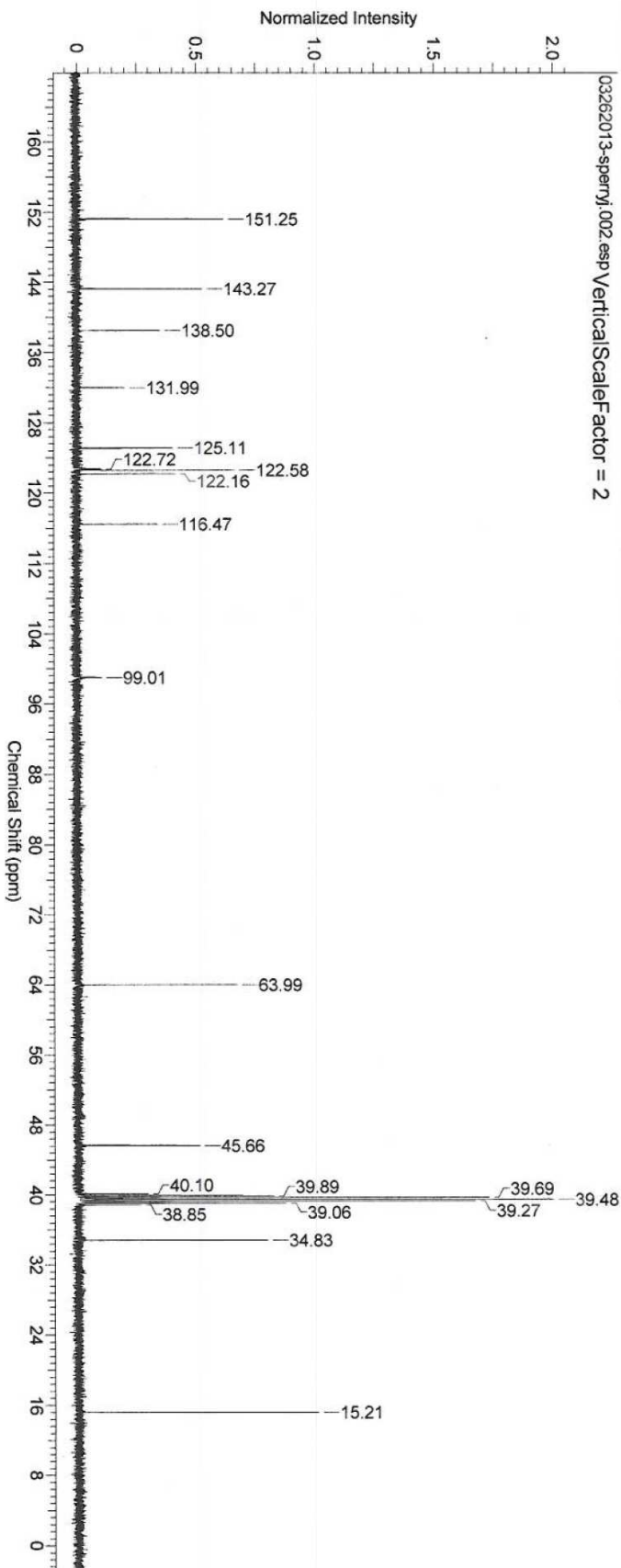


| No. | (ppm)          | Annotation | Layer No. | Created By | Created At               | Modified By | Modified At |
|-----|----------------|------------|-----------|------------|--------------------------|-------------|-------------|
| 1   | [2.49 .. 2.53] | DMSO       | 1         | sperryj    | Tue 3/26/2013 1:42:47 PM |             |             |

| No. | (ppm)         | Value      | Absolute Value | Non-Negative Value | No. | (ppm)         | Value      | Absolute Value | Non-Negative Value |
|-----|---------------|------------|----------------|--------------------|-----|---------------|------------|----------------|--------------------|
| 1   | 9119 .. 0.992 | 94742060   | 4.79765965e+9  | 2.94742060         | 7   | 7117 .. 6.821 | 0.0134218  | 1.62993318e+9  | 1.00134218         |
| 2   | 8143 .. 1.991 | 0.03782618 | 1.68932006e+9  | 1.03782618         | 8   | 8655 .. 7.080 | 99398077   | 1.61795072e+9  | 0.99398077         |
| 3   | 8953 .. 3.020 | 99632889   | 1.62177293e+9  | 0.99632889         | 9   | 2945 .. 7.391 | 0.1458180  | 1.65148403e+9  | 1.01458180         |
| 4   | 1491 .. 3.291 | 0.6419969  | 1.73224947e+9  | 1.06419969         | 10  | 8893 .. 7.801 | 0.1079679  | 1.64532301e+9  | 1.01079679         |
| 5   | 3465 .. 3.462 | 0.4132581  | 3.32276506e+9  | 2.04132581         | 11  | 8209 .. 7.941 | 0.1099491  | 1.64564557e+9  | 1.01099491         |
| 6   | 5215 .. 4.661 | 0.1364422  | 1.64995789e+9  | 1.01364422         | 12  | 2026 .. 8.431 | 0.02947557 | 1.67572736e+9  | 1.02947557         |

Number of Nuclei 0 C's

|                        |                                                            |                        |                                                          |
|------------------------|------------------------------------------------------------|------------------------|----------------------------------------------------------|
| Acquisition Time (sec) | 1.3631                                                     | Comment                | 705714-021-01 13C C13CPD_day DMSO /opt/topspin spenry 23 |
| Date                   | 26 Mar 2013 13:29:36                                       | Date Stamp             | 26 Mar 2013 13:29:36                                     |
| File Name              | \seg\IO\data\BH091709\data\spenry\nmr\03262013-spenry\2fid |                        |                                                          |
| Nucleus                | 13C                                                        | Number of Transients   | 256                                                      |
| Owner                  | nmr                                                        | Points Count           | 32768                                                    |
| SW(cyclical) (Hz)      | 24038.46                                                   | Solvent                | DMSO-d6                                                  |
| Sweep Width (Hz)       | 24037.73                                                   | Temperature (degree C) | 22.600                                                   |
| Origin                 | spec                                                       | Pulse Sequence         | zgpg30                                                   |
| Spectrum Offset (Hz)   | 10010.4990                                                 | Spectrum Type          | STANDARD                                                 |
| Original Points Count  | 32768                                                      | Receiver Gain          | 203.00                                                   |
| Frequency (MHz)        | 100.61                                                     |                        |                                                          |



| No. | (ppm) | (Hz)   | Height | No. | (ppm) | (Hz)   | Height | No. | (ppm)  | (Hz)    | Height |
|-----|-------|--------|--------|-----|-------|--------|--------|-----|--------|---------|--------|
| 1   | 15.21 | 1530.5 | 1.0100 | 7   | 39.69 | 3993.2 | 1.7289 | 13  | 116.47 | 11718.7 | 0.3390 |
| 2   | 34.83 | 3504.6 | 0.7992 | 8   | 39.89 | 4013.7 | 0.8251 | 14  | 122.16 | 12290.9 | 0.4136 |
| 3   | 38.85 | 3908.8 | 0.2653 | 9   | 40.10 | 4035.0 | 0.2963 | 15  | 122.58 | 12333.4 | 0.6640 |
| 4   | 39.06 | 3930.1 | 0.8757 | 10  | 45.66 | 4594.0 | 0.5135 | 16  | 122.72 | 12347.4 | 0.1053 |
| 5   | 39.27 | 3951.4 | 1.6716 | 11  | 63.99 | 6438.3 | 0.6722 | 17  | 125.11 | 12588.0 | 0.4029 |
| 6   | 39.48 | 3971.9 | 2.0000 | 12  | 99.01 | 9961.7 | 0.1042 | 18  | 131.99 | 13279.8 | 0.2024 |
|     |       |        |        |     |       |        |        | 19  | 138.50 | 13934.9 | 0.3511 |
|     |       |        |        |     |       |        |        | 20  | 143.27 | 14414.6 | 0.5277 |
|     |       |        |        |     |       |        |        | 21  | 151.25 | 15217.2 | 0.6179 |