

Analysis of the binding of Mixed Lineage Leukemia 1 (MLL1) and Histone 3 peptides to WD Repeat Domain 5 (WDR5) for the design of inhibitors targeting

MLL1-WDR5 interaction

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Supporting Information

Table S1----- S2-S3

Table S1. Characterization data of synthesized peptides.

| Peptide | % Purity analytical RP-(HPLC)* | Calculated | Observed (ESI-MS)** |
|------------------------|-----------------------------------|---------------|------------------------|
| | | $(M+2H)^{2+}$ | |
| WIN-FAM-1 | > 99 | 1026.009 | 1026.20 |
| WIN-FAM-2 | 99 | 1032.538 | 1032.60 |
| | | $(M+H)^+$ | |
| 10mer-Ala-FAM | 98 | 1920.013 | 1919.87 |
| 10mer-Thr-FAM | 99 | 1950.024 | 1949.87 |
| WIN | 95 | 1351.756 | 1351.73 |
| Ac-11mer | > 99 | 1294.734 | 1294.80 |
| Ac-10mer | 90 | 1207.702 | 1207.73 |
| NH ₂ -11mer | > 99 | 1252.724 | 1252.80 |
| Ac- 9mer | 98 | 1136.665 | 1136.73 |
| Ac-7mer | 96 | 836.474 | 836.53 |
| Ac-6mer | 97 | 723.390 | 723.53 |
| Ac-5mer | 99 | 586.331 | 586.47 |
| Ac-4mer | 93 | 487.263 | 487.40 |
| Ac-3mer | 96 | 358.220 | 358.33 |
| Ac-2mer | > 99 | 287.183 | 287.27 |
| NH ₂ -10mer | 98 | 1165.692 | 1165.73 |
| | | | |

| | | | |
|----------------------------|------|----------|---------|
| NH ₂ -3mer | > 99 | 316.210 | 316.27 |
| CHO-ARA | > 99 | 344.205 | 344.27 |
| Δ1 | > 99 | 372.236 | 372.33 |
| Δ2a | 95 | 372.236 | 372.33 |
| Δ2b | > 99 | 386.252 | 386.33 |
| Δ2c | 95 | 373.220 | 373.33 |
| H3-10mer | > 99 | 1145.687 | 1145.80 |
| Ac-H3-10mer | > 99 | 1187.697 | 1187.73 |
| H3-3mer | 93 | 346.220 | 346.27 |
| Ac-H3-3mer | 95 | 388.231 | 388.33 |
| H3-10mer-K4Me | > 99 | 1159.702 | 1159.80 |
| H3-10mer-K4Me ₂ | > 99 | 1173.718 | 1173.80 |
| H3-10mer-K4Me ₃ | > 99 | 1188.741 | 1187.80 |

* Waters, Sunfire™ C18, 4.6×150mm, 5μm.

** Finnigan LCQ Deca (Thermoquest).