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|                                         |                                                                 |                       |
|-----------------------------------------|-----------------------------------------------------------------|-----------------------|
| Empirical formula                       | $\text{C}_{15}\text{H}_{18}\text{N}_2\text{O}_3$                |                       |
| Formula weight                          | 274.31                                                          |                       |
| Temperature                             | 294(2) K                                                        |                       |
| Wavelength                              | 0.71073 Å                                                       |                       |
| Crystal system                          | Orthorhombic                                                    |                       |
| Space group                             | $P2_12_12_1$                                                    |                       |
| Unit cell dimensions                    | $a = 6.348(3)$ Å                                                | $\alpha = 90^\circ$ . |
|                                         | $b = 9.402(4)$ Å                                                | $\beta = 90^\circ$ .  |
|                                         | $c = 47.10(2)$ Å                                                | $\gamma = 90^\circ$ . |
| Volume                                  | $2811(2)$ Å <sup>3</sup>                                        |                       |
| Z                                       | 8                                                               |                       |
| Density (calculated)                    | $1.296 \text{ Mg/m}^3$                                          |                       |
| Absorption coefficient                  | $0.091 \text{ mm}^{-1}$                                         |                       |
| F(000)                                  | 1168                                                            |                       |
| Crystal size                            | $0.400 \times 0.320 \times 0.220 \text{ mm}^3$                  |                       |
| $\theta$ range for data collection      | $2.333$ to $28.308^\circ$ .                                     |                       |
| Index ranges                            | $-7 \leq h \leq 8$ , $-5 \leq k \leq 12$ , $-62 \leq l \leq 48$ |                       |
| Reflections collected                   | 15836                                                           |                       |
| Independent reflections                 | 6953 [ $R(\text{int}) = 0.0345$ ]                               |                       |
| Completeness to $\theta = 25.242^\circ$ | 99.4 %                                                          |                       |
| Refinement method                       | Full-matrix least-squares on $F^2$                              |                       |
| Data / restraints / parameters          | 6953 / 0 / 371                                                  |                       |
| Goodness-of-fit on $F^2$                | 0.979                                                           |                       |
| Final R indices [ $I > 2\sigma(I)$ ]    | $R1 = 0.0600$ , $wR2 = 0.1495$                                  |                       |
| R indices (all data)                    | $R1 = 0.1117$ , $wR2 = 0.1733$                                  |                       |
| Absolute structure parameter            | 0.1(5)                                                          |                       |
| Largest diff. peak and hole             | $0.145$ and $-0.188 \text{ e.Å}^{-3}$                           |                       |
| Measurement                             | Bruker D8 QUEST PHOTON-100 Detector                             |                       |
| Software Used                           | SHELXTL-PLUS                                                    |                       |

Figure 1

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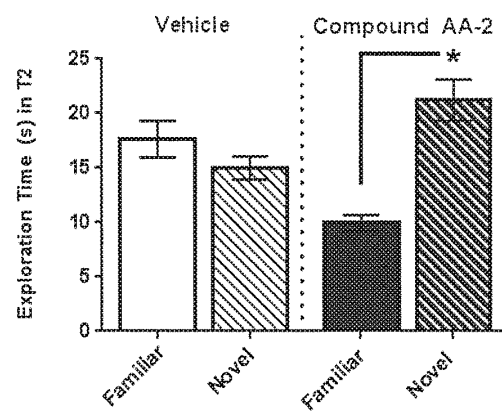


Figure 2A

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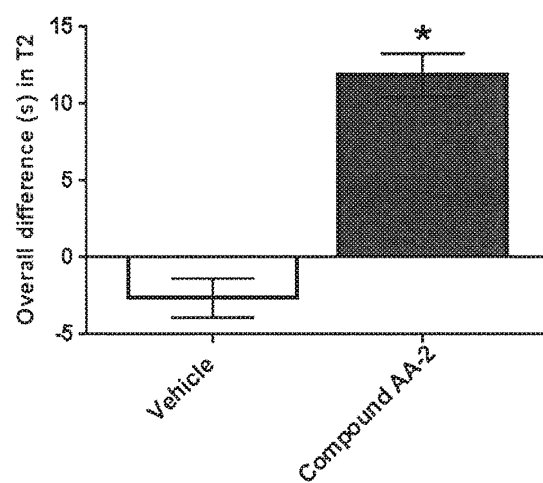


Figure 2B

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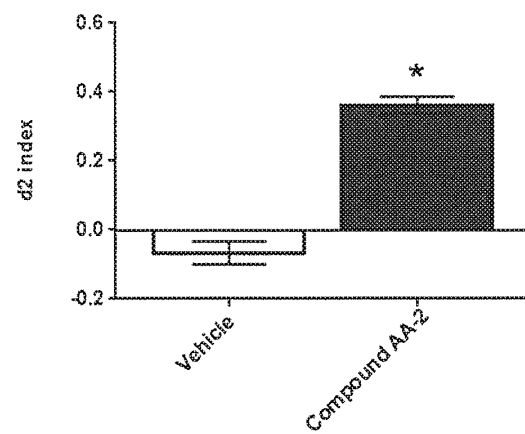


Figure 2C