

Table S2. Information of PonAAS2 inhibitors found by the initial screening.

	molecular formula	molecular weight	concentration ( $\mu\text{M}$ ) <sup>1</sup>	
HTS09643	C <sub>15</sub> H <sub>11</sub> NO <sub>6</sub> S	333.3	120.0	
HTS09784	C <sub>13</sub> H <sub>20</sub> N <sub>6</sub> O	276.3	144.7	
HTS10037	C <sub>14</sub> H <sub>17</sub> NO <sub>3</sub>	247.3	161.7	
HTS10442	C <sub>12</sub> H <sub>9</sub> NO <sub>4</sub>	231.2	173.0	
HTS10550	C <sub>16</sub> H <sub>13</sub> N <sub>3</sub> O <sub>2</sub>	279.3	143.2	
HTS11483	C <sub>11</sub> H <sub>10</sub> CIN <sub>3</sub>	219.7	182.1	
HTS12813	C <sub>12</sub> H <sub>9</sub> N <sub>3</sub> OS	243.3	164.4	
HTS12892	C <sub>11</sub> H <sub>9</sub> NO <sub>2</sub> S	219.3	182.4	
JA00082	C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub>	166.1	240.8	
JFD03671	C <sub>16</sub> H <sub>11</sub> N <sub>3</sub> O	261.3	153.1	
JFD03939	C <sub>9</sub> H <sub>6</sub> INO <sub>4</sub> S	351.1	113.9	

<sup>1</sup> Concentrations of compounds in the reaction used in the first screening were shown as  $\mu\text{M}$ .