Supplemental File

Design, Synthesis and Evaluation of Guanylhyazones as Potentials Inhibitors or Reactivators of Acetylcholinesterase

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IR, HRMS (ESI), MS (ESI), ¹H AND ¹³C NMR spectra

Pralidoxime (2-PAM) (1)

MS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

1-methylpyridine-2-carboxaldehyde hydrazone (2)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

1-methylpyridine-2-carboxaldehyde guanylhydrazone (3)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

Pyridine-2-carboxaldehyde guanylhyazone (4)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

benzaldehyde guanylhydrazone (5)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

4-nitrobenzaldehyde guanylhydrazone (6)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

4-chlorobenzaldehyde guanyldiazide (7)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

4-methylbenzaldehyde guanyldiazide (8)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

4-dimethylaminobenzaldehyde guanylhydrazone (9)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

4-hydroxybenzaldehyde guanyldiazide (10)

IR

HRMS (ES+)

¹H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

2,4-dinitrobenzaldehyde guanyldiazide (11)

IR

MS (ES+)

^1H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

2,4-dichlorobenzaldehyde guanylhyazone (12)

IR

MS (ES⁺)

^1H NMR (300 MHz, DMSO)

^{13}C NMR (75 MHz, DMSO)

NMR TEST – SPECTRA WITH 5 MINUTES

NMR TEST – SPECTRA WITH 20 MINUTES

NMR TEST – SPECTRA WITH 40 MINUTES

NMR TEST – SPECTRA WITH 100 MINUTES (METHYL GROUP INTEGRATION OF SUBSTRATE AND AChE)

Inhibition curve of compound 1-methylpyridine-2-carboxaldehyde hydrazine (2)

Inhibition curve of compound 4-nitrobenzaldehyde guanylhyazone (6)

Inhibition curve of compound 2,4-dinitrobenzaldehyde guanylhyazone (11)