

DMD #50831

R.L. Myette, G. Conseil, S.P. Ebert, B. Wetzel, M.R. Detty, S.P.C. Cole Drug Metab. Dispos.
“Chalcogenopyrylium Dyes as Differential Modulators of Organic Anion Transport by MRP1,
MRP2 and MRP4”

Supplemental TABLE 1

Chemical names and quantum fluorescence of CGPs studied

CGP Class	Chemical Name	Quantum Fluorescence ¹
I-1	2,4-di(4- <i>N,N</i> -dimethylaminophenyl)-6-methylselenopyrylium chloride	$\Phi_F < 0.001$
I-2	2,4-di(4- <i>N,N</i> -dimethylaminophenyl)-6-butylthiopyrylium bromide	$\Phi_F < 0.001$
I-3	2,4-di(4- <i>N,N</i> -dimethylaminophenyl)-6- <i>tert</i> -butylthiopyrylium iodide	$\Phi_F < 0.001$
I-4	2,4-di(4- <i>N,N</i> -dimethylaminophenyl)-6- <i>tert</i> -butylselenopyrylium chloride	$\Phi_F < 0.001$
I-5	2,4-di(4- <i>N,N</i> -dimethylaminophenyl)-6- <i>tert</i> -butyltelluropyrylium bromide	$\Phi_F < 0.001$
II-1	2,6-di- <i>tert</i> -butyl-4-phenylthiopyrylium bromide	$\Phi_F < 0.005$
II-2	2,6-di- <i>tert</i> -butyl-4-phenylselenopyrylium bromide	$\Phi_F < 0.005$
II-3	2,6-di- <i>tert</i> -butyl-4-phenyltelluropyrylium bromide	$\Phi_F < 0.005$
II-4	2,6-di- <i>tert</i> -butyl-4-(5-carboxythien-2-yl)thiopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-5	2,6-di- <i>tert</i> -butyl-4-(5-carboxythien-2-yl)selenopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-6	2,6-di- <i>tert</i> -butyl-4-(5-carboxythien-2-yl)telluropyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-7	2,6-di- <i>tert</i> -butyl-4-(phenyl-2- <i>N,N</i> -diethylcarboxamido)thiopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-8	2,6-di- <i>tert</i> -butyl-4-(phenyl-2- <i>N,N</i> -diethylcarboxamido)selenopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-9	2,6-di- <i>tert</i> -butyl-4-(phenyl-2- <i>N,N</i> -diethylcarboxamido)telluropyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-10	2,6-di- <i>tert</i> -butyl-4-methylselenopyrylium hexafluorophosphate	$\Phi_F < 0.005$

II-11	2,6-di- <i>tert</i> -butyl-4-methylpyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-12	2,6-diphenyl-4-methylthiopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-13	2,6-di- <i>tert</i> -butyl-4-(<i>N</i> -piperidyl-2-thienyl-5-thiocarboxamido)thiopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-14	2,6-di- <i>tert</i> -butyl-4-(<i>N</i> -piperidyl-2-thienyl-5-thiocarboxamido)selenopyrylium hexafluorophosphate	$\Phi_F < 0.005$
II-15	2,6-di- <i>tert</i> -butyl-4-(<i>N</i> -piperidyl-2-thienyl-5-thiocarboxamido)telluropyrylium hexafluorophosphate	$\Phi_F < 0.005$
III-1	2- <i>tert</i> -butyl-6-(4- <i>N,N</i> -dimethylaminophenyl)-4-(<i>N</i> -piperidyl-2-thienyl-5-thiocarboxamido)thiopyrylium chloride	$\Phi_F < 0.005$
III-2	2- <i>tert</i> -butyl-6-(4- <i>N,N</i> -dimethylaminophenyl)-4-(5-carboxythien-2-yl)thiopyrylium hexafluorophosphate	$\Phi_F < 0.005$
III-3	2- <i>tert</i> -butyl-6-(4- <i>N,N</i> -dimethylaminophenyl)-4-(phenyl-2- <i>N,N</i> -diethylcarboxamido)thiopyrylium chloride	$\Phi_F < 0.005$
III-4	2- <i>tert</i> -butyl-4-phenyl-6-(4- <i>N,N</i> -dimethylaminophenyl)thiopyrylium hexafluorophosphate	$\Phi_F < 0.005$
IV-1	2-phenyl-6-(4-aminophenyl)-4-(4- <i>N</i> -morpholinophenyl)telluropyrylium hexafluorophosphate	$\Phi_F < 0.001$
IV-2	2,6-di(4-aminophenyl)-4-(4- <i>N</i> -morpholinophenyl)telluropyrylium hexafluorophosphate	$\Phi_F < 0.001$
IV-3	2-(4-aminophenyl)-4,6-di(4- <i>N</i> -morpholinophenyl)telluropyrylium hexafluorophosphate	$\Phi_F < 0.001$
V-1	4-((2,6-diphenyl-4 <i>H</i> -telluropyran-4-ylidene)methyl)-2,6-diphenyltelluropyrylium	$\Phi_F < 0.001$
V-2	4-((2,6-di- <i>tert</i> -butyl-4 <i>H</i> -selenopyran-4-ylidene)methyl)-2,6-di- <i>tert</i> -butylselenopyrylium	$\Phi_F = 0.0055$
V-3	4-((2,6-di- <i>tert</i> -butyl-4 <i>H</i> -selenopyran-4-ylidene)methyl)-2,6-di- <i>tert</i> -butylpyrylium trifluoromethanesulfonate	$\Phi_F = 0.008$

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V-4	4-((2,6-di- <i>tert</i> -butyl-4 <i>H</i> -telluropyran-4-ylidene)methyl)-2,6-di- <i>tert</i> -butylpyrylium hexafluorophosphate	$\Phi_F = 0.005$
V-5	4-((2,6-di- <i>tert</i> -butyl-4 <i>H</i> -telluropyran-4-ylidene)methyl)-2,6-di- <i>tert</i> -butylthiopyrylium	$\Phi_F = 0.0014$
V-6	4-(2-((2,6-di- <i>tert</i> -butyl-4 <i>H</i> -selenopyran-4-ylidene)methyl)ethenyl)-2,6-di- <i>tert</i> -butylselenopyrylium	$\Phi_F = 0.0024$
V-7	4-(2-((2,6-di- <i>tert</i> -butyl-4 <i>H</i> -telluropyran-4-ylidene)methyl)ethenyl)-2,6-di- <i>tert</i> -butylpyrylium	$\Phi_F < 0.005$

¹All compounds have little or no fluorescence. For values listed as “ $\Phi_F < 0.001$ ”, no emission signal was detected at all; for values listed as “ $\Phi_F < 0.005$ ”, a signal above background was detected, but could not be quantified.

Detty MR; Merkel PB. Chalcogenopyrylium dyes as potential photochemotherapeutic agents. III. Solution studies of heavy atom effects on triplet yields, Quantum efficiencies of singlet oxygen generation, rates of reaction with singlet oxygen, and emission quantum yields. *J. Am. Chem. Soc.* **1990**, *112*, 3845-3855.

Ohulchanskyys TY; Gannon MK II; Ye M; Wagner S J; Skripchenko A; Prasad PN; Detty MR. “Switched-on” flexible chalcogenopyrylium photosensitizers upon binding to DNA. Purging of viral pathogens through singlet-oxygen induced DNA cleavage. *J. Phys. Chem. B* **2007**, *111*, 9686-9692.