Supporting Information

Inhibition of Group IVA cytosolic phospholipase A_2 by thiazolyl ketones *in vitro*, *ex vivo*, and *in vivo*

George Kokotos,[*†] *Astrid J. Feuerherm*[‡,§] *Efrosini Barbayianni*[‡,†] *Ishita Shah,*[#] *Mari Sæther,*[§] *Victoria Magrioti,*[†] *Thuy Nguyen,*[§] *Violetta Constantinou-Kokotou,*[‖] *Edward A. Dennis,*[#] *and Berit Johansen**[§]

[‡]A.J.F. and E.B. contributed equally to this work.
[†]Laboratory of Organic Chemistry, Department of Chemistry, University of Athens, Panepistimiopolis, Athens 15771, Greece.
[§]Department of Biology, NTNU, University of Trondheim, Trondheim, Norway.
[#]Department of Chemistry and Biochemistry and Department of Pharmacology, School of Medicine, University of California, San Diego, La Jolla, California 92093-0601.
[‖]Chemical Laboratories, Agricultural University of Athens, Athens 11855, Greece.

*To whom correspondence should be addressed. For G.K.: phone: +30 210 7274462; fax: +30 210 7274761; E-mail: gkokotos@chem.uoa.gr. *For B.J.: phone: +47 73598691; E-mail: berit.johansen@ntnu.no

Contents

Table S1. Names and code numbers of tested compounds.

Compound chemical name	No	Code number
2-Phenoxy-1-(thiazol-2-yl)ethanone	**13a**	GK245
2-(4-Fluorophenoxy)-1-(thiazol-2-yl)ethanone	**13b**	GK247
2-(Biphenyl-4-yloxy)-1-(thiazol-2-yl)ethanone	**18a**	GK246
2-(4-Octylphenoxy)-1-(thiazol-2-yl)ethanone	**18b**	GK185
1-(Benzo[d]thiazol-2-yl)-2-(4-octylphenoxy)ethanone	**18c**	GK191
Ethyl 2-(2-(2-(4-octylphenoxy)acetyl)thiazol-4-yl)acetate	**24a**	GK203
Ethyl 2-(2-(2-(dodecyloxy)acetyl)thiazol-4-yl)acetate	**24b**	GK230
Ethyl 2-(2-(dodecyloxy)acetyl)thiazole-4-carboxylate	**24c**	GK229
Methyl 2-(2-(4-octylphenoxy)acetyl)thiazole-4-carboxylate	**28**	GK470

Table S2. Elemental analyses of synthesized compounds.

Compound No	Molecular Formula	Calculated	Found
13a	$C_{11}H_9NO_2S$	C, 60.26; H, 4.14; N, 6.39	C, 60.14; H, 4.21; N, 6.33
13b	$C_{11}H_8FNO_2S$	C, 55.69; H, 3.40; N, 5.90	C, 55.43; H, 3.47; N, 5.81
15b	$C_{18}H_{28}O_3$	C, 73.93; H, 9.65	C, 73.85; H, 9.81
16a	$C_{14}H_{14}O_2$	C, 78.48; H, 6.59	C, 78.22; H, 6.73
16b	$C_{16}H_{26}O_2$	C, 76.75; H, 10.47	C, 76.58; H, 10.62
17a	$C_{17}H_{15}NO_2S$	C, 68.66; H, 5.08; N, 4.71	C, 68.43; H, 5.24; N, 4.52
17b	$C_{19}H_{27}NO_2S$	C, 68.43; H, 8.16; N, 4.20	C, 68.21; H, 8.33; N, 4.15
17c	$C_{23}H_{29}NO_2S$	C, 72.02; H, 7.62; N, 3.65	C, 71.90; H, 7.74; N, 3.55
18a	$C_{17}H_{13}NO_2S$	C, 69.13; H, 4.44; N, 4.74	C, 69.02; H, 4.53; N, 4.60
18b	$C_{19}H_{25}NO_2S$	C, 68.85; H, 7.60; N, 4.23	C, 68.76; H, 7.71; N, 4.12
18c	$C_{23}H_{27}NO_2S$	C, 72.40; H, 7.13; N, 3.67	C, 72.23; H, 7.22; N, 3.61
20a	$C_{23}H_{39}NO_2Si$	C, 70.90; H, 10.09; N, 3.59	C, 70.78; H, 10.16; N, 3.52
20b	$C_{21}H_{43}NO_2Si$	C, 68.23; H, 11.72; N, 3.79	C, 68.45; H, 11.83; N, 3.73
21a	$C_{23}H_{41}NO_3Si$	C, 67.76; H, 10.14; N, 3.44	C, 67.55; H, 10.26; N, 3.37
21b	$C_{21}H_{45}NO_3Si$	C, 65.06; H, 11.70; N, 3.61	C, 64.88; H, 11.85; N, 3.52
22a	$C_{23}H_{41}NO_2SSi$	C, 65.19; H, 9.75; N, 3.31	C, 65.01; H, 9.84; N, 3.25
22b	$C_{21}H_{45}NO_2SSi$	C, 62.47; H, 11.23; N, 3.47	C, 62.25; H, 11.34; N, 3.39
23a	$C_{23}H_{33}NO_4S$	C, 65.84; H, 7.93; N, 3.34	C, 65.73; H, 8.01; N, 3.25
23b	$C_{21}H_{37}NO_4S$	C, 63.12; H, 9.33; N, 3.51	C, 63.01; H, 9.43; N, 3.44
23c	$C_{20}H_{35}NO_4S$	C, 62.30; H, 9.15; N, 3.63	C, 62.14; H, 9.26; N, 3.57
24a	$C_{23}H_{31}NO_4S$	C, 66.16; H, 7.48; N, 3.35	C, 66.02; H, 7.54; N, 3.26
24b	$C_{21}H_{35}NO_4S$	C, 63.44; H, 8.87; N, 3.52	C, 63.28; H, 8.99; N, 3.43
24c	$C_{20}H_{33}NO_4S$	C, 62.63; H, 8.67; N, 3.65	C, 62.41; H, 8.79; N, 3.55
25	$C_{27}H_{45}NO_4SSi$	C, 63.86; H, 8.93; N, 2.76	C, 63.72; H, 9.04; N, 2.68
26	$C_{27}H_{43}NO_4SSi$	C, 64.12; H, 8.57; N, 2.77	C, 63.97; H, 8.68; N, 2.69

27	$C_{21}H_{29}NO_4S$	C, 64.42; H, 7.47; N, 3.58	C, 64.13; H, 7.61; N, 3.48
28	$C_{21}H_{27}NO_4S$	C, 64.75; H, 6.99; N, 3.60	C, 64.66; H, 7.07; N, 3.51

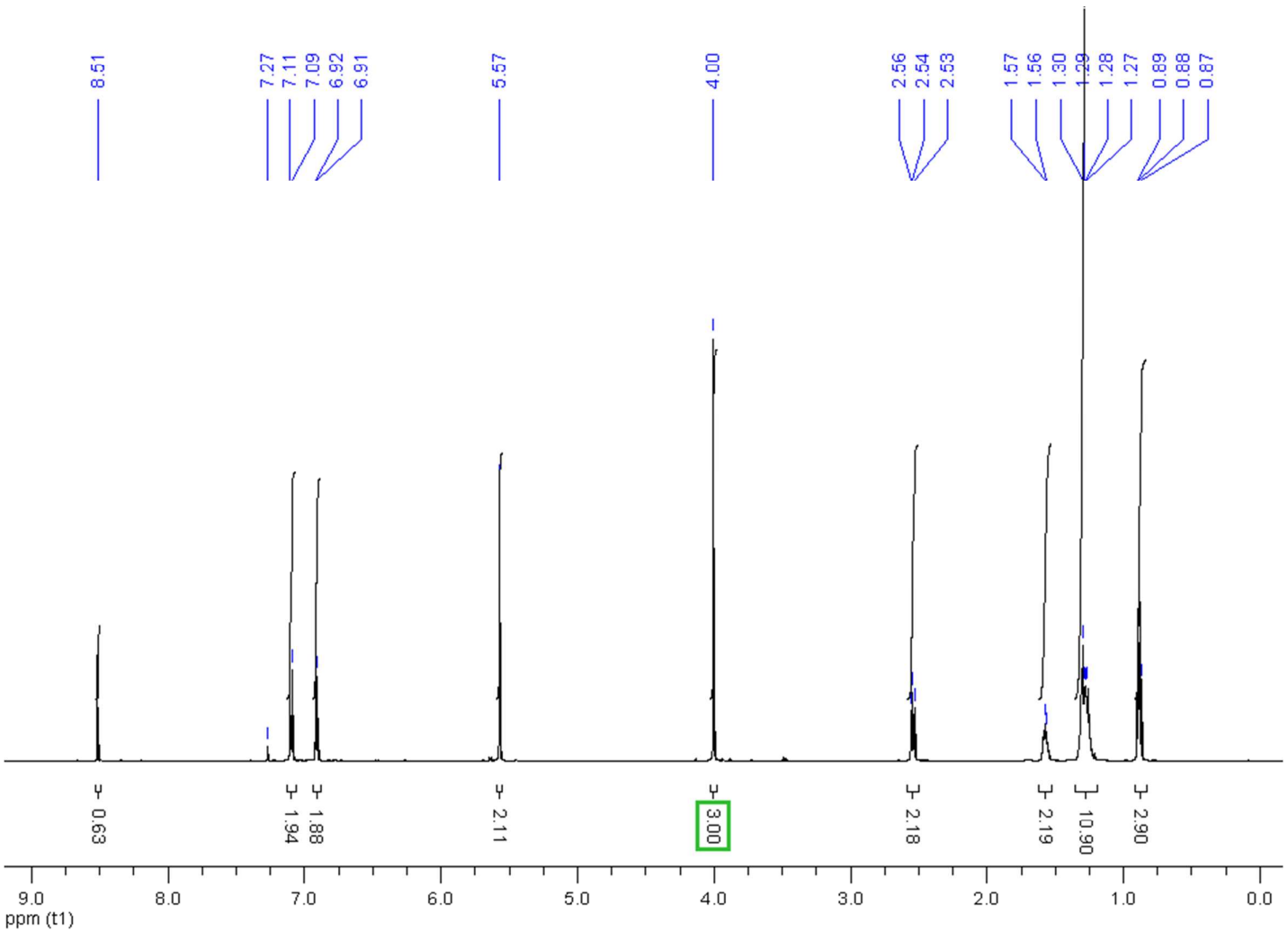


Figure S1. ^{1}H NMR (600 MHz) spectrum of inhibitor **28** in $CDCl_3$.

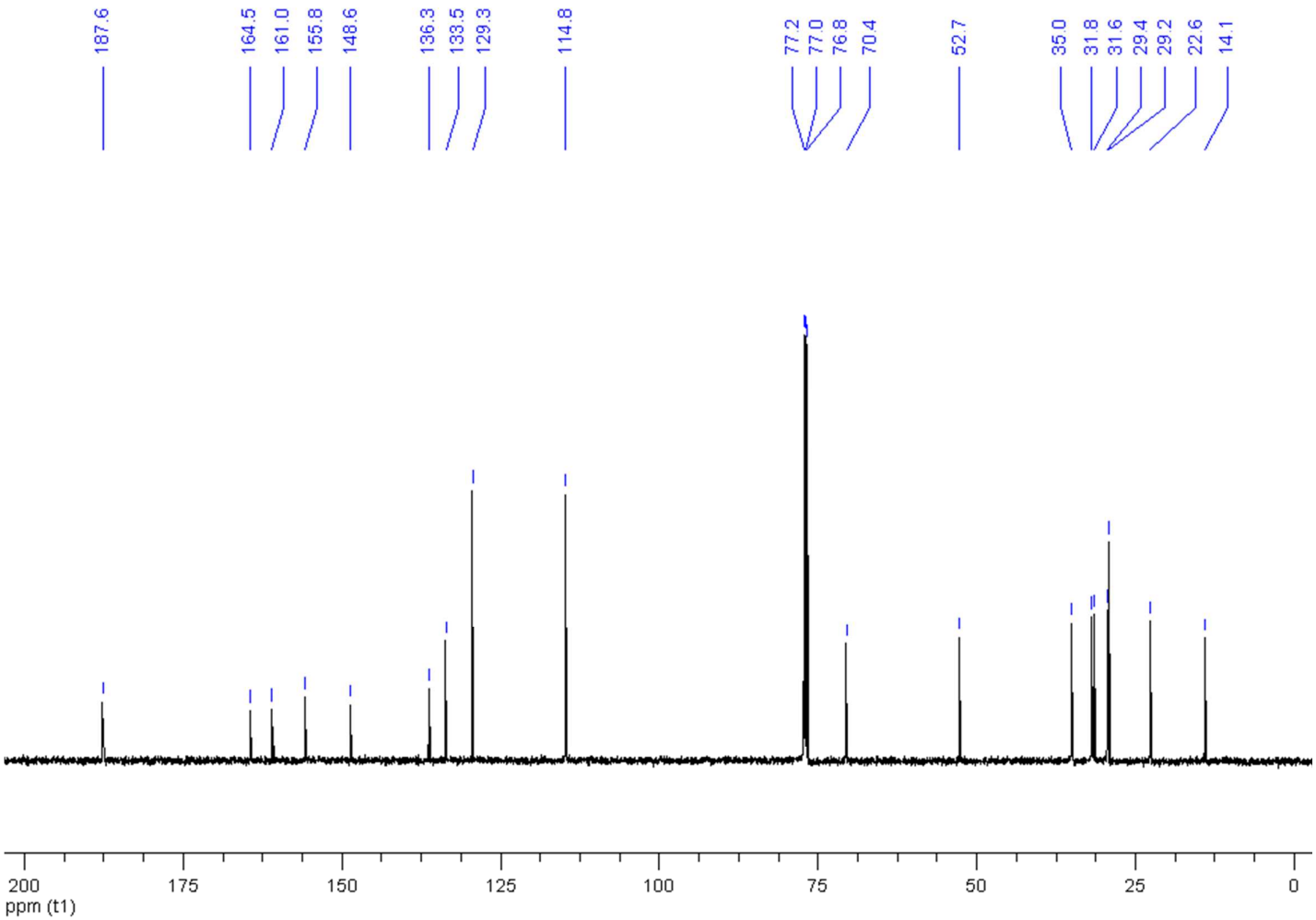
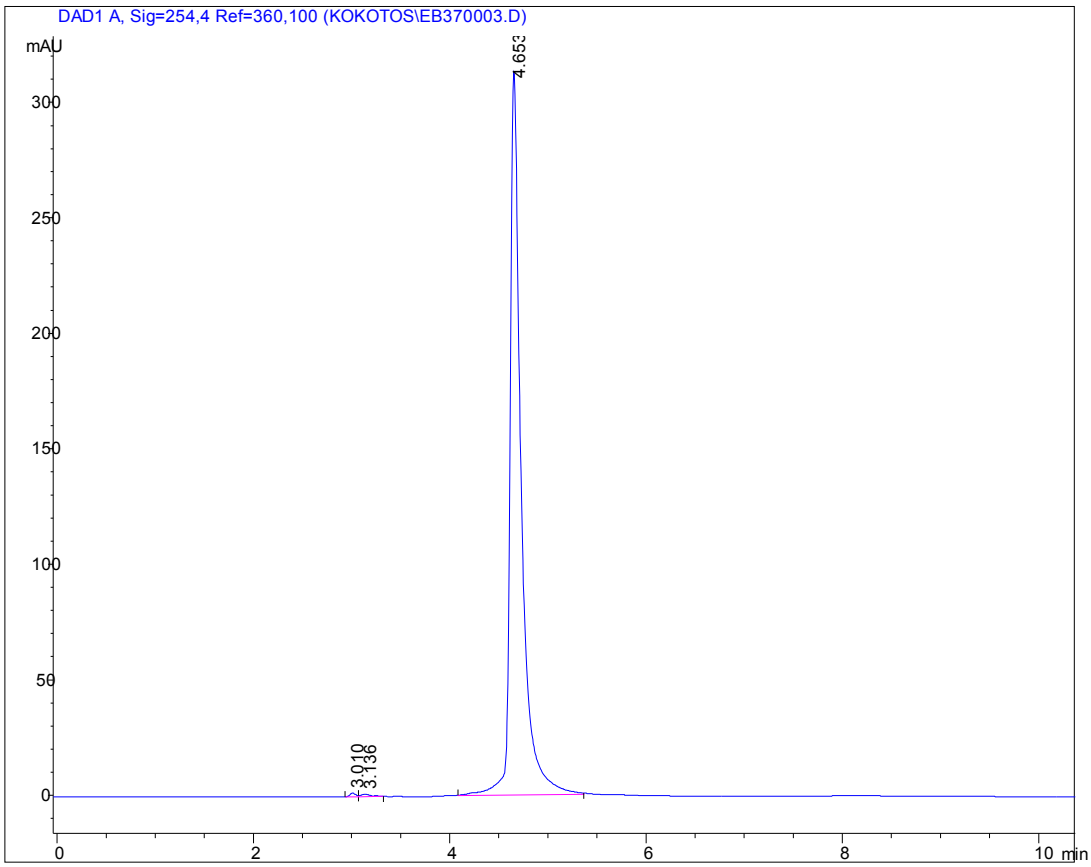


Figure S2. ^{13}C NMR (150 MHz) spectrum of inhibitor **28** in $CDCl_3$.



Signal 1: DAD1 A, Sig=254,4 Ref=360,100

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.010	PV	0.0651	6.62785	1.57495	0.2643
2	3.136	VB	0.1131	7.39787	1.01426	0.2950
3	4.653	BB	0.1147	2493.42261	313.67416	99.4406
Totals :				2507.44832	316.26337	

Figure S3: HPLC chromatogram of inhibitor **28** [hexane/i-propanol 9:1, 1 mL/min, column: Thermo Scientific, Hypersil Silica, 250×4.6 (5μM)].