

Table S1. Characterization data of novel synthetic compounds

Compound no.	$[\alpha]_D^a$	c (g/dL)	temp.	Formula	HRMS (MH) ^{+b}	
					Calcd.	Found
7	+2.02	0.248	25.3	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3740
8	-41.13	0.282	25.3	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3755
9	-1.71	0.234	25.4	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3726
10	-34.71	0.265	27.0	C ₄₃ H ₅₃ N ₁₁ O ₆ F	838.4164	838.4180
11	-61.71	0.222	26.9	C ₃₆ H ₄₇ N ₁₁ O ₅ Cl	748.3450	748.3444
12	-51.79	0.139	26.8	C ₃₆ H ₄₇ N ₁₁ O ₅ Br	792.2945	792.2939
13	-41.11	0.090	26.9	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3734
14	-53.52	0.213	26.9	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3752
15^c				C ₃₅ H ₄₆ N ₁₁ O ₅	700.3683	700.3691
16	-60.87	0.161	24.3	C ₃₄ H ₄₆ N ₁₁ O ₅ S	720.3404	720.3412
18	-33.97	0.259	25.2	C ₃₆ H ₄₇ N ₁₁ O ₅ Cl	748.3450	748.3458
19	-35.16	0.236	25.2	C ₃₆ H ₄₇ N ₁₁ O ₅ Br	792.2945	792.2955
20	-58.02	0.212	25.0	C ₃₆ H ₄₇ N ₁₂ O ₇	759.3691	759.3680
21	-52.24	0.245	25.0	C ₃₆ H ₄₈ N ₁₁ O ₆	730.3789	730.3776
22	-53.27	0.214	25.2	C ₃₆ H ₄₉ N ₁₂ O ₅	729.3949	729.3962
23	-12.59	0.127	25.2	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3726
24	-38.43	0.281	25.1	C ₃₆ H ₄₇ N ₁₁ O ₅ F	732.3746	732.3753
25	-138.89	0.036	24.8	C ₄₀ H ₄₇ N ₈ O ₆	735.3619	735.3622
26^d	-66.66	0.243	25.2	C ₃₈ H ₄₃ N ₈ O ₆	707.3306	707.3300
27^d	-79.81	0.327	25.4	C ₃₈ H ₄₃ N ₈ O ₆	707.3306	707.3313
28	-58.61	0.301	25.4	C ₃₆ H ₄₃ N ₁₀ O ₆	711.3367	711.3364
29	-42.42	0.198	25.4	C ₃₆ H ₄₃ N ₁₀ O ₆	711.3367	711.3359
30	-61.25	0.214	27.0	C ₃₆ H ₄₃ N ₁₀ O ₆	711.3367	711.3378
31	-54.95	0.134	26.3	C ₃₆ H ₄₃ N ₉ O ₆	692.2945	692.2941
32	-44.53	0.119	25.1	C ₃₃ H ₄₆ N ₁₃ O ₅	704.3745	704.3750
33	-36.56	0.134	24.0	C ₃₃ H ₄₆ N ₁₃ O ₅	704.3745	704.3738
34	-47.18	0.267	25.1	C ₃₄ H ₄₆ N ₁₁ O ₅ S	720.3404	720.3417
35	-39.48	0.157	24.7	C ₃₉ H ₄₉ N ₁₂ O ₅	765.3949	765.3964
36	-42.44	0.278	25.5	C ₃₇ H ₅₀ N ₁₁ O ₅	728.3996	728.4012
37^c				C ₃₅ H ₄₆ N ₁₁ O ₅	700.3683	700.3676
38	-63.77	0.196	26.6	C ₃₆ H ₄₂ N ₁₀ O ₅ F	713.3324	713.3317
39	-45.02	0.191	26.8	C ₃₆ H ₄₂ N ₁₀ O ₅ F	713.3324	713.3320
40	-51.78	0.224	26.9	C ₃₆ H ₃₇ N ₉ O ₅ F	694.2902	694.2893
41	-69.54	0.174	27.0	C ₃₆ H ₄₂ N ₁₀ O ₅ F	713.3324	713.3336
42	-32.81	0.259	27.0	C ₃₆ H ₄₂ N ₁₀ O ₅ F	713.3324	713.3312
43	-65.57	0.183	27.0	C ₃₆ H ₃₇ N ₉ O ₅ F	694.2902	694.2907

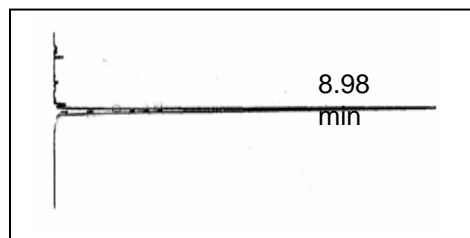
^aOptical rotations were measured in H₂O with a Horiba high-sensitive polarimeter SEPA-200 (Kyoto, Japan).

^bExact mass (HRMS) spectra were recorded on a JEOLJMS-01SG -2 or JMS-HX/HX 110A mass spectrometer.

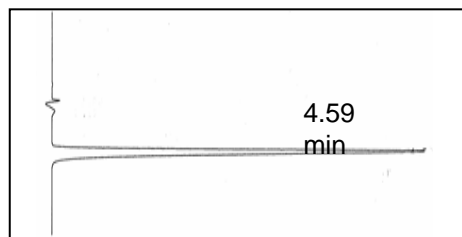
^cCompounds **15** and **37** were prepared as racemic mixtures containing L/D-Phg since HPLC peaks of the corresponding diastereomers were proximate.

^dThe structures of compounds **26** and **27** were determined tentatively by yields of HPLC separation in the synthesis using Fmoc-L-Phg-OH.

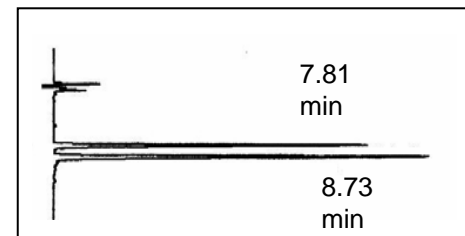
Compd. 7 H₂O/CH₃CN = 78 : 22



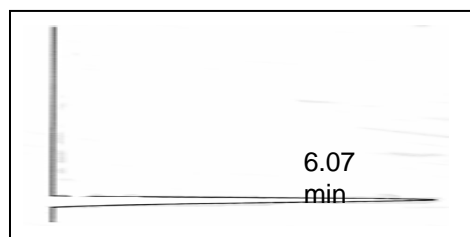
Compd. 11 H₂O/CH₃CN = 69 : 31



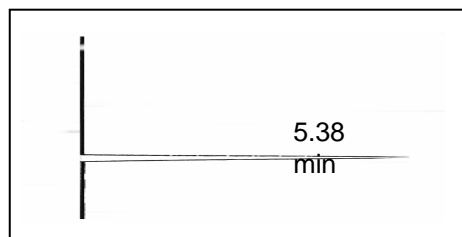
Compd. 15 H₂O/CH₃CN = 72 : 28



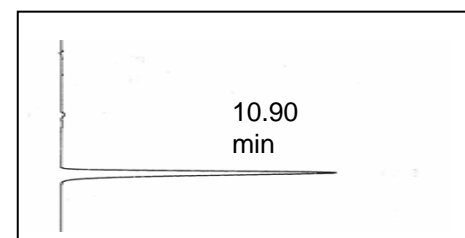
Compd. 8 H₂O/CH₃CN = 72 : 28



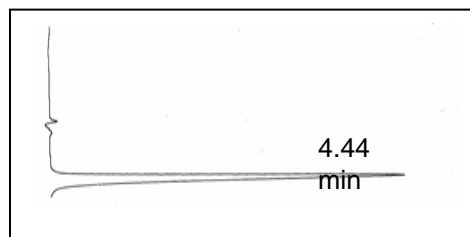
Compd. 12 H₂O/CH₃CN = 70 : 30



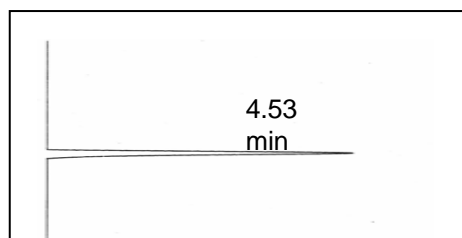
Compd. 16 H₂O/CH₃CN = 76 : 24



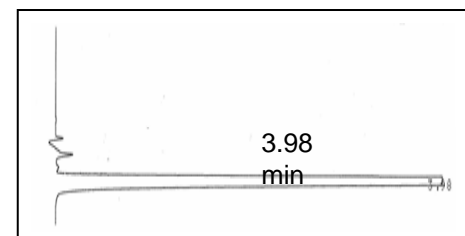
Compd. 9 H₂O/CH₃CN = 68 : 32



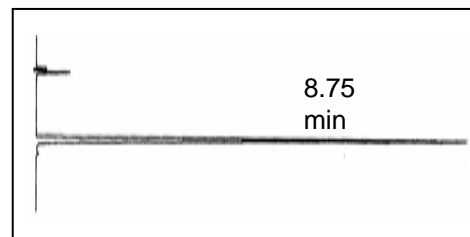
Compd. 13 H₂O/CH₃CN = 71 : 29



Compd. 18 H₂O/CH₃CN = 72 : 28



Compd. 10 H₂O/CH₃CN = 64 : 36



Compd. 14 H₂O/CH₃CN = 71 : 29



Compd. 19 H₂O/CH₃CN = 79 : 21

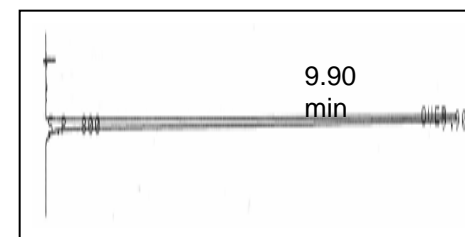
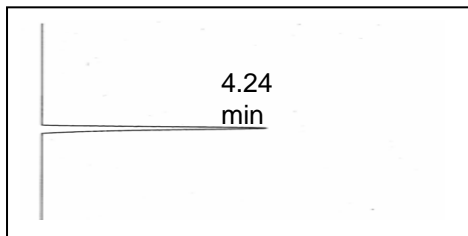


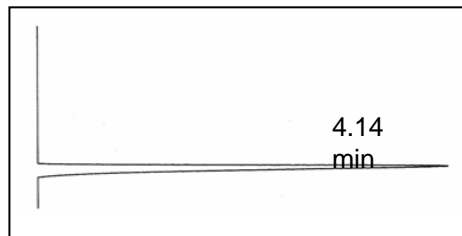
Fig. S1. HPLC charts of purified samples of novel synthetic compounds 7-19.

HPLC solvents were H₂O and CH₃CN, both containing 0.1% (v/v) TFA. A Cosmosil 5C18-AR column (4.6 × 250 mm, Nacalai Tesque Inc., Kyoto, Japan) was eluted with an isocratic mode (shown above each HPLC profile) at a flow rate of 1 mL/min on a Shimadzu LC-10ADvp (Shimadzu corporation, Ltd., Kyoto, Japan).

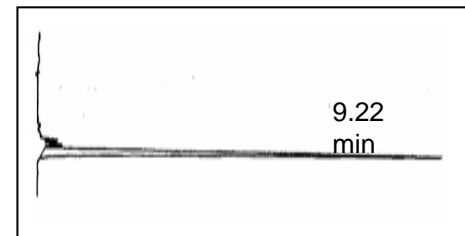
Compd. 20 H₂O/CH₃CN = 73 : 27



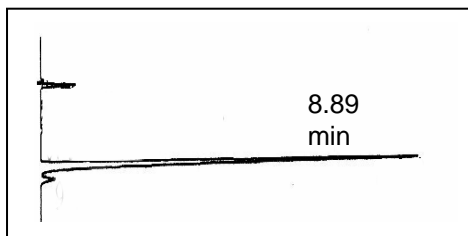
Compd. 24 H₂O/CH₃CN = 74 : 26



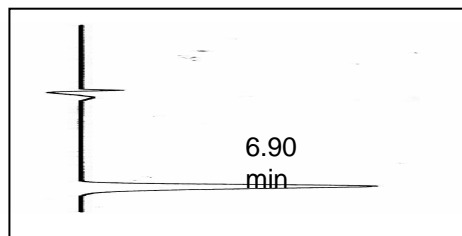
Compd. 28 H₂O/CH₃CN = 71 : 29



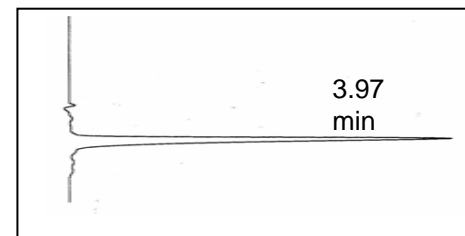
Compd. 21 H₂O/CH₃CN = 78 : 22



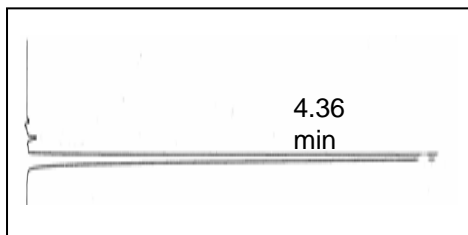
Compd. 25 H₂O/CH₃CN = 66 : 34



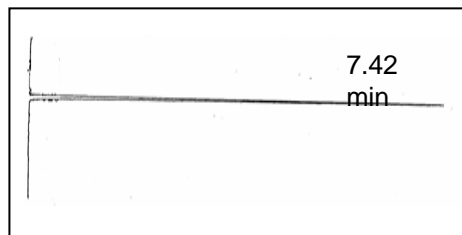
Compd. 29 H₂O/CH₃CN = 76 : 24



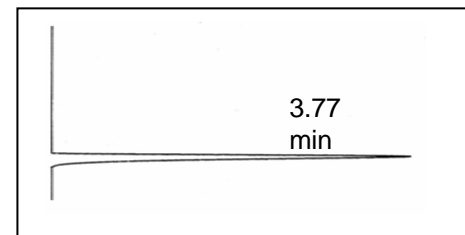
Compd. 22 H₂O/CH₃CN = 77 : 23



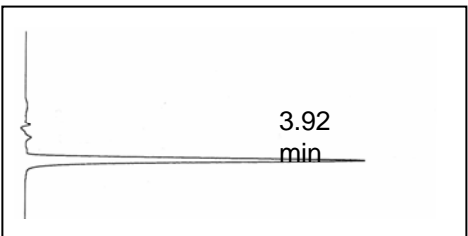
Compd. 26 H₂O/CH₃CN = 72 : 28



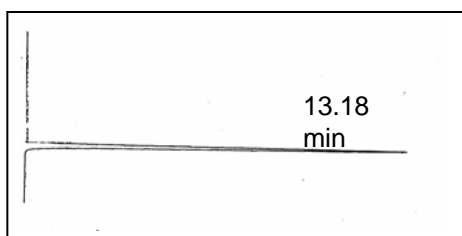
Compd. 30 H₂O/CH₃CN = 72 : 28



Compd. 23 H₂O/CH₃CN = 74 : 26



Compd. 27 H₂O/CH₃CN = 72 : 28



Compd. 31 H₂O/CH₃CN = 71 : 29

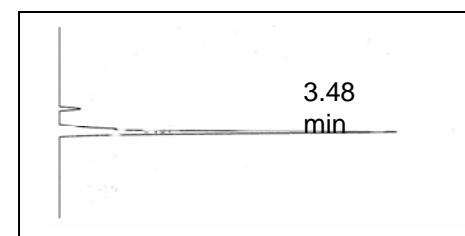
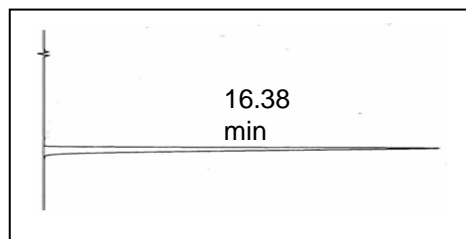
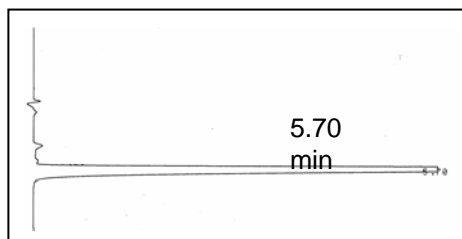


Fig. S2. HPLC charts of purified samples of novel synthetic compounds **20-31**. HPLC solvents were H₂O and CH₃CN, both containing 0.1% (v/v) TFA. A Cosmosil 5C18-AR column (4.6 × 250 mm, Nacalai Tesque Inc., Kyoto, Japan) was eluted with an isocratic mode (shown above each HPLC profile) at a flow rate of 1 mL/min on a Shimadzu LC-10ADvp (Shimadzu corporation, Ltd., Kyoto, Japan).

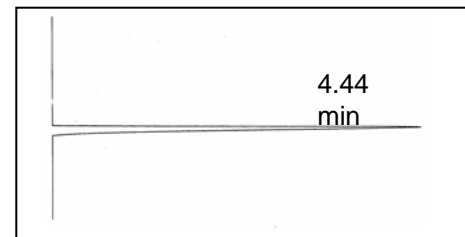
Compd. 32 H₂O/CH₃CN = 82 : 18



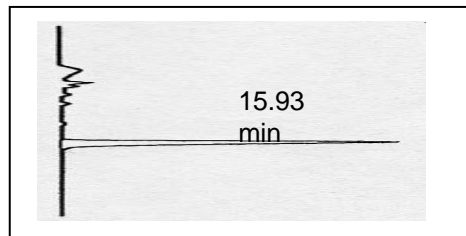
Compd. 36 H₂O/CH₃CN = 73 : 27



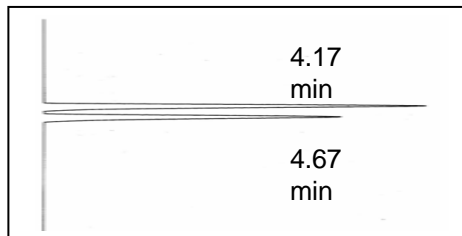
Compd. 40 H₂O/CH₃CN = 71 : 29



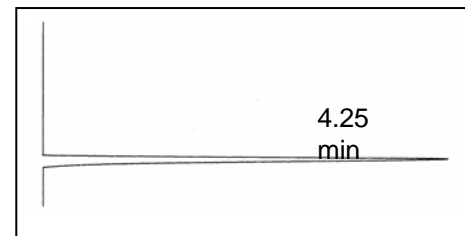
Compd. 33 H₂O/CH₃CN = 80 : 20



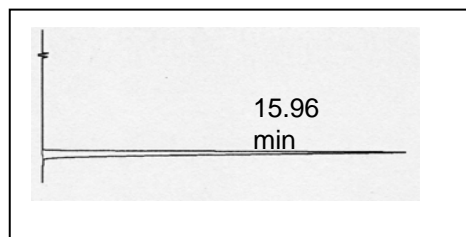
Compd. 37 H₂O/CH₃CN = 75 : 25



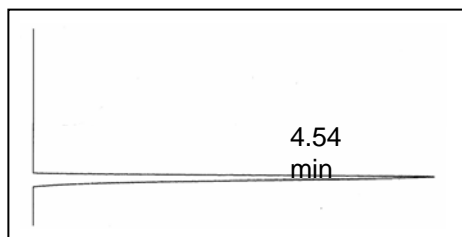
Compd. 41 H₂O/CH₃CN = 73 : 27



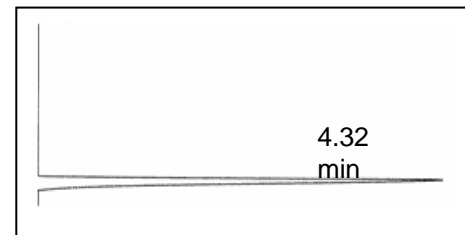
Compd. 34 H₂O/CH₃CN = 79 : 21



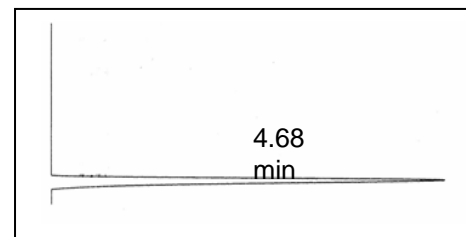
Compd. 38 H₂O/CH₃CN = 71 : 29



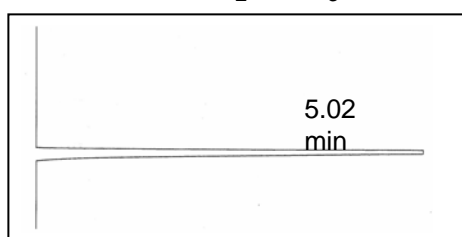
Compd. 42 H₂O/CH₃CN = 74 : 26



Compd. 35 H₂O/CH₃CN = 72 : 28



Compd. 39 H₂O/CH₃CN = 72 : 28



Compd. 43 H₂O/CH₃CN = 74 : 26

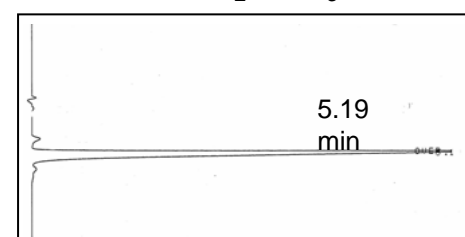


Fig. S3. HPLC charts of purified samples of novel synthetic compounds **32-43**. HPLC solvents were H₂O and CH₃CN, both containing 0.1% (v/v) TFA. A Cosmosil 5C18-AR column (4.6 × 250 mm, Nacalai Tesque Inc., Kyoto, Japan) was eluted with an isocratic mode (shown above each HPLC profile) at a flow rate of 1 mL/min on a Shimadzu LC-10ADvp (Shimadzu corporation, Ltd., Kyoto, Japan).