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	$C_{36}H_{47}N_{11}O_5F$	732.3746	732.3740
8	-41.13	0.282	25.3	$C_{36}H_{47}N_{11}O_5F$	732.3746	732.3755
9	-1.71	0.234	25.4	$C_{36}H_{47}N_{11}O_5F$	732.3746	732.3726
10	-34.71	0.265	27.0	$C_{43}H_{53}N_{11}O_6F$	838.4164	838.4180
11	-61.71	0.222	26.9	$C_{36}H_{47}N_{11}O_5Cl$	748.3450	748.3444
12	-51.79	0.139	26.8	$C_{36}H_{47}N_{11}O_5Br$	792.2945	792.2939
13	-41.11	0.090	26.9	$C_{36}H_{47}N_{11}O_5F$	732.3746	732.3734
14	-53.52	0.213	26.9	$C_{36}H_{47}N_{11}O_5F$	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	$C_{34}H_{46}N_{11}O_5S$	720.3404	720.3412
18	-33.97	0.259	25.2	$C_{36}H_{47}N_{11}O_5Cl$	748.3450	748.3458
19	-35.16	0.236	25.2	$C_{36}H_{47}N_{11}O_5Br$	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	$C_{36}H_{47}N_{11}O_5F$	732.3746	732.3726
24	-38.43	0.281	25.1	$C_{36}H_{47}N_{11}O_5F$	732.3746	732.3753
25	-138.89	0.036	24.8	$C_{40}H_{47}N_8O_6$	735.3619	735.3622
26[d]	-66.66	0.243	25.2	$C_{38}H_{43}N_8O_6$	707.3306	707.3300
27[d]	-79.81	0.327	25.4	$C_{38}H_{43}N_8O_6$	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	$C_{36}H_{43}N_9O_6$	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	$C_{34}H_{46}N_{11}O_5S$	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	$C_{36}H_{42}N_{10}O_5F$	713.3324	713.3317
39	-45.02	0.191	26.8	$C_{36}H_{42}N_{10}O_5F$	713.3324	713.3320
40	-51.78	0.224	26.9	$C_{36}H_{37}N_9O_5F$	694.2902	694.2893
41	-69.54	0.174	27.0	$C_{36}H_{42}N_{10}O_5F$	713.3324	713.3336
42	-32.81	0.259	27.0	$C_{36}H_{42}N_{10}O_5F$	713.3324	713.3312
43	-65.57	0.183	27.0	$C_{36}H_{37}N_9O_5F$	694.2902	694.2907

[a]Optical rotations were measured in H_2O with a Horiba high-sensitive polarimeter SEPA-200 (Kyoto, Japan).
[b]Exact mass (HRMS) spectra were recorded on a JEOLJMS-01SG -2 or JMS-HX/HX 110A mass spectrometer.
[c]Compounds **15** and **37** were prepared as racemic mixtures containing L/D-Phg since HPLC peaks of the corresponding diasteomers were proximate.
[d]The structures of compounds **26** and **27** were determined tentatively by yields of HPLC separation in the synthesis using Fmoc-L-Phg-OH.

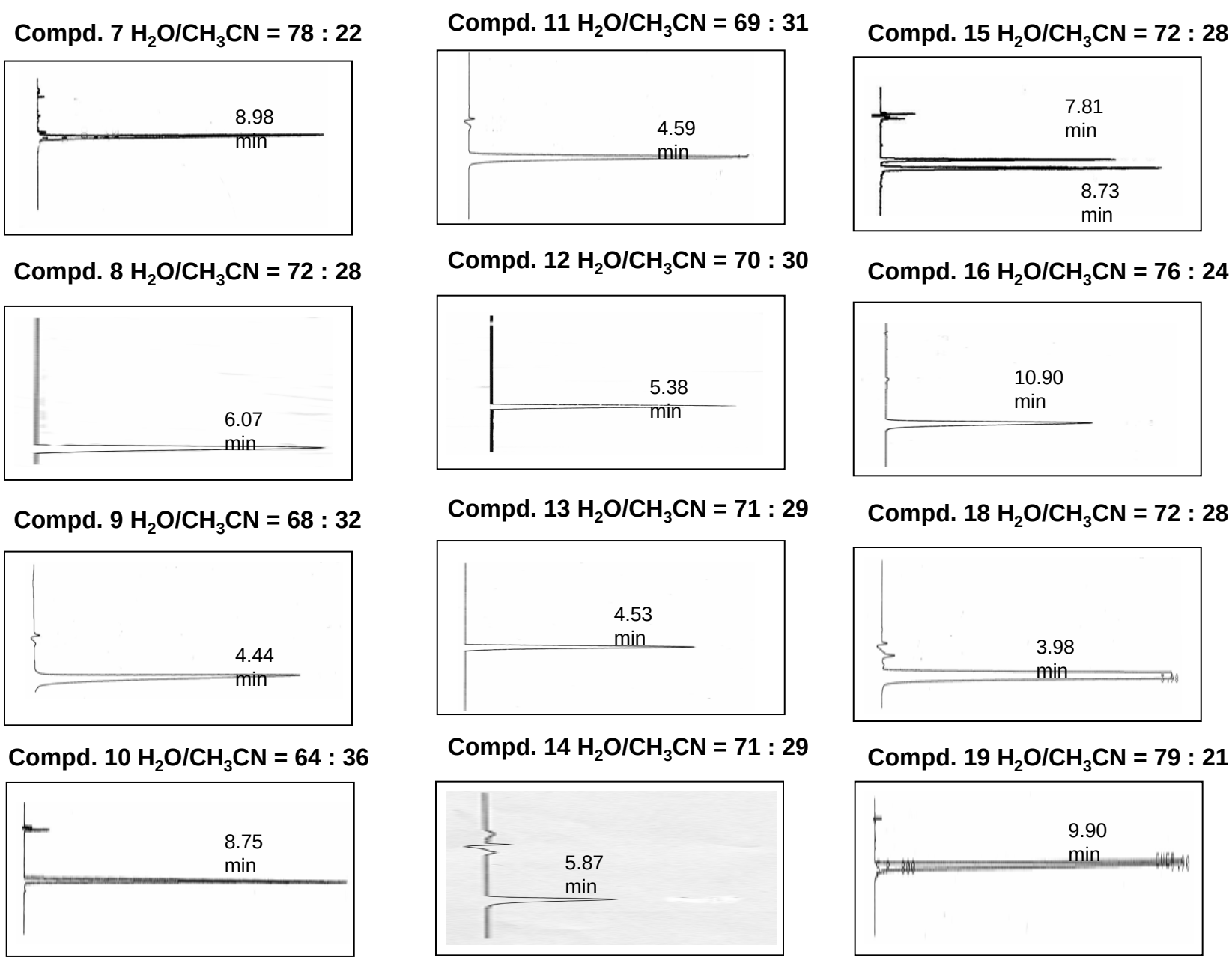

Fig. S1. HPLC charts of purified samples of novel synthetic compounds **7**-**19**.
HPLC solvents were H_2O and CH_3CN, both containing 0.1% (v/v) TFA. A Cosmosil 5C18-AR column (4.6 × 250 mm, Nacalai Tesque Inc., Kyoto, Japan) was eluted with an isocratic mode (shown above each HPLC profile) at a flow rate of 1 mL/min on a Shimadzu LC-10ADvp (Shimadzu corporation, Ltd., Kyoto, Japan).

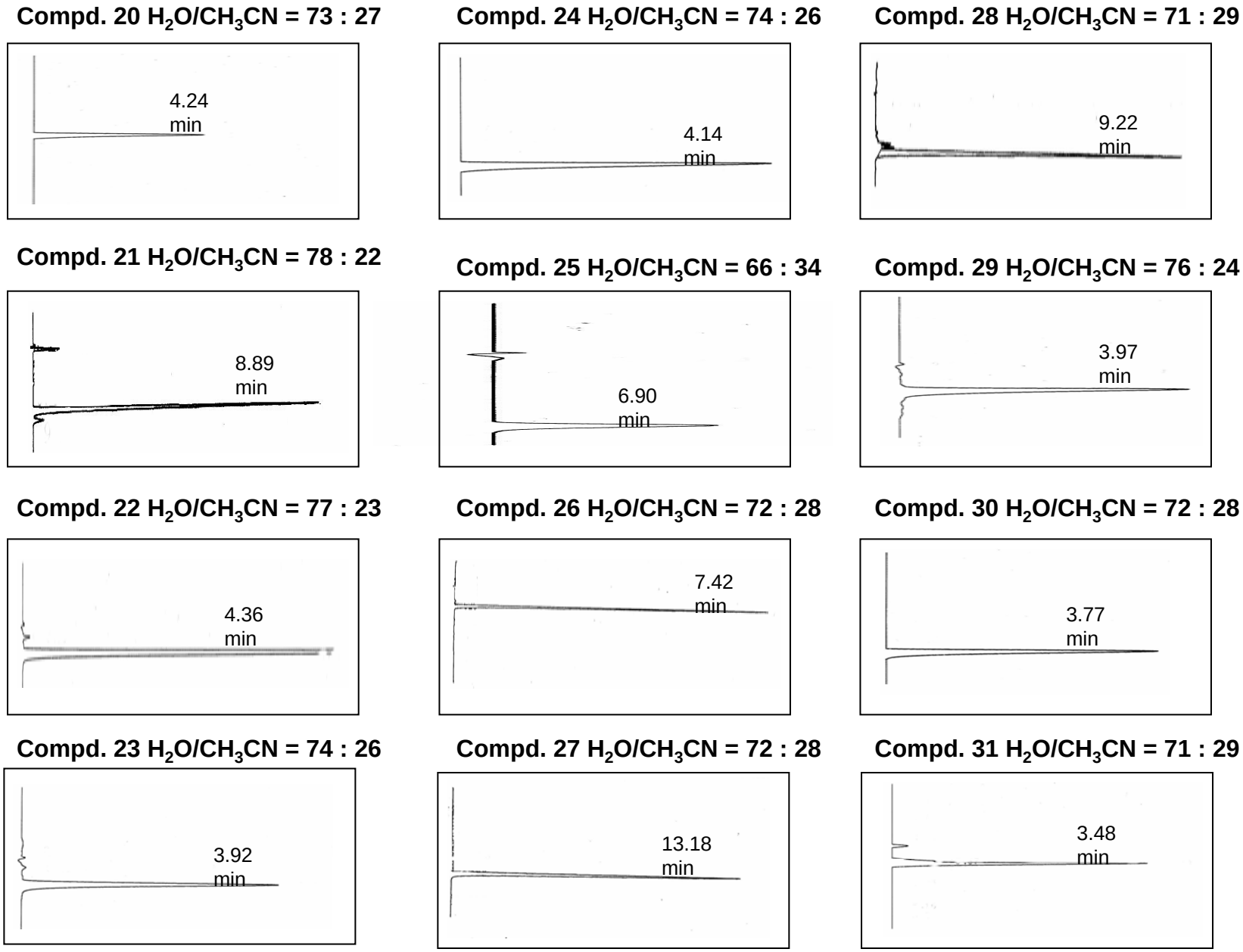

Fig. S2. HPLC charts of purified samples of novel synthetic compounds **20**-**31**.
HPLC solvents were H_2O and CH_3CN, both containing 0.1% (v/v) TFA. A Cosmosil 5C18-AR column (4.6 × 250 mm, Nacalai Tesque Inc., Kyoto, Japan) was eluted with an isocratic mode (shown above each HPLC profile) at a flow rate of 1 mL/min on a Shimadzu LC-10ADvp (Shimadzu corporation, Ltd., Kyoto, Japan).

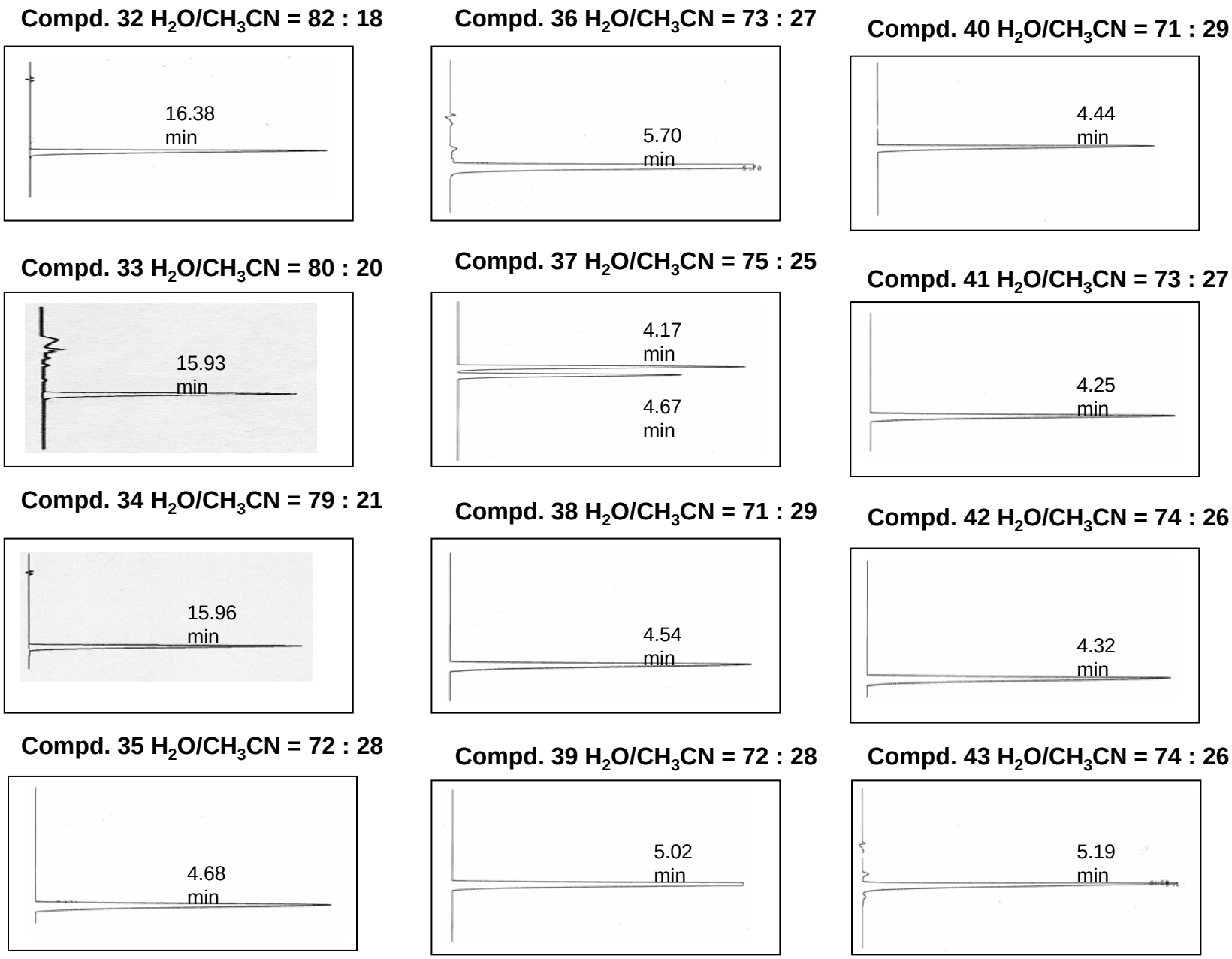

Fig. S3. HPLC charts of purified samples of novel synthetic compounds **32**-**43**.
HPLC solvents were H_2O and CH_3CN, both containing 0.1% (v/v) TFA. A Cosmosil 5C18-AR column (4.6 × 250 mm, Nacalai Tesque Inc., Kyoto, Japan) was eluted with an isocratic mode (shown above each HPLC profile) at a flow rate of 1 mL/min on a Shimadzu LC-10ADvp (Shimadzu corporation, Ltd., Kyoto, Japan).