Supplementary data for article:

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Supporting information

Consensus based comparison of chromatographic and computational estimated lipophilicity of benzothiepino[3,2-c]pyridine derivatives as potential antifungal drugs

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Table S1. Retention parameters (R_F) of dibenzo[*b*,*f*]thiepines in typical reversed-phase and microemulsion chromatographic systems.

Comp. No.	Typical reversed-phase TLC																MELC-TLC	
	Organic modifier																	
	Acetone						Methanol					Dioxane					MELC1	MELC2
	90%	85%	80%	75%	70%	65%	98%	94%	90%	86%	82%	85%	80%	75%	70%	65%		
1	0.63	0.62	0.57	0.52	0.48	0.41	0.53	0.48	0.46	0.44	0.4	0.84	0.75	0.71	0.62	0.37	0.30	0.43
2	0.73	0.62	0.50	0.35	0.28	0.17	0.56	0.47	0.44	0.36	0.28	0.77	0.67	0.60	0.49	0.25	0.29	0.40
3	0.59	0.50	0.42	0.29	0.23	0.14	0.45	0.36	0.32	0.27	0.18	0.74	0.64	0.53	0.37	0.16	0.27	0.37
4	0.58	0.46	0.40	0.23	0.19	0.08	0.37	0.26	0.23	0.17	0.13	0.76	0.64	0.50	0.32	0.11	0.23	0.33
5	0.64	0.52	0.44	0.26	0.24	0.12	0.44	0.34	0.32	0.24	0.17	0.78	0.66	0.51	0.35	0.14	0.21	0.31
6	0.66	0.53	0.46	0.29	0.24	0.12	0.42	0.32	0.30	0.23	0.14	0.82	0.70	0.53	0.39	0.16	0.21	0.31
7	0.66	0.51	0.45	0.25	0.22	0.09	0.48	0.38	0.35	0.26	0.18	0.78	0.67	0.51	0.37	0.15	0.21	0.30
8	0.66	0.55	0.51	0.35	0.33	0.21	0.50	0.42	0.41	0.35	0.25	0.83	0.76	0.60	0.46	0.23	0.26	0.37
9	0.64	0.50	0.45	0.29	0.27	0.14	0.46	0.38	0.35	0.29	0.20	0.79	0.69	0.53	0.42	0.22	0.22	0.32
10	0.63	0.47	0.41	0.22	0.21	0.08	0.43	0.31	0.28	0.20	0.14	0.76	0.66	0.49	0.34	0.17	0.19	0.30
11	0.63	0.45	0.41	0.24	0.18	0.11	0.42	0.30	0.28	0.20	0.15	0.78	0.67	0.52	0.32	0.19	0.23	0.33
12	0.64	0.47	0.42	0.25	0.21	0.10	0.35	0.24	0.21	0.15	0.12	0.82	0.69	0.52	0.35	0.15	0.23	0.33
13	0.73	0.53	0.46	0.31	0.11	0.11	0.53	0.41	0.39	0.29	0.20	0.88	0.74	0.57	0.37	0.18	0.22	0.32
14	0.67	0.50	0.42	0.27	0.22	0.09	0.42	0.29	0.26	0.18	0.14	0.77	0.68	0.53	0.36	0.16	0.23	0.33
15	0.76	0.56	0.48	0.31	0.25	0.10	0.53	0.42	0.39	0.3	0.24	0.83	0.74	0.57	0.43	0.15	0.24	0.33
16	0.75	0.58	0.56	0.39	0.35	0.23	0.49	0.42	0.39	0.33	0.26	0.76	0.72	0.62	0.52	0.25	0.30	0.39
17	0.71	0.56	0.53	0.33	0.32	0.22	0.54	0.46	0.43	0.39	0.28	0.72	0.70	0.56	0.47	0.21	0.31	0.40

Table S2a. *In silico* estimated log*P* values and solubility parameter of benzothiepino[3,2-c]pyridine derivtaves.

Comp. No	miLogP	KOWWIN	AlogPs	AClogP	AlogP	MLOGP	XlogP2	XlogP3	AlogpS*
1	2.66	2.70	2.14	2.29	1.80	1.51	1.90	2.34	-2.83
2	3.75	3.73	3.54	3.37	2.95	2.60	3.15	3.14	-4.05
3	4.41	4.37	4.15	3.98	3.62	3.19	3.78	4.04	-4.64
4	5.52	5.49	5.24	5.05	4.47	3.91	5.09	5.04	-6.29
5	5.48	5.49	5.33	4.40	4.43	3.91	5.01	4.59	-5.67
6	5.53	5.57	5.23	4.30	4.42	3.53	4.93	4.56	-5.67
7	5.64	5.69	5.27	4.46	4.64	4.30	5.17	4.69	-5.38
8	5.23	5.04	4.67	4.21	4.31	3.46	4.74	4.31	-4.89
9	4.49	4.62	4.44	4.06	3.41	3.32	3.87	3.82	-4.70
10	5.65	6.02	5.13	5.45	4.78	4.45	5.27	5.20	-5.61
11	5.48	5.49	5.34	4.40	4.43	3.91	5.01	4.59	-5.65
12	5.58	5.57	4.92	4.95	4.46	3.53	5.01	5.01	-6.25
13	5.40	5.57	4.81	5.26	4.66	3.99	4.99	4.92	-4.75
14	5.53	5.57	5.22	4.30	4.42	3.53	4.93	4.56	-5.70
15	5.28	5.04	4.68	4.86	4.35	3.46	4.82	4.76	-4.96
16	3.79	3.81	3.48	3.26	2.94	2.31	3.07	3.39	-4.14
17	2.92	3.93	3.50	3.43	3.16	3.06	3.32	3.52	-3.78

*Data are estimated solubilities

Table S2b. Chromatographic lipophilicty descriptors of benzothiepino[3,2-c]pyridine derivtaves.

Comp. No.	R_M^0_MeOH	*b*_MeOH	*PC1*_MeOH	C_0_MeOH	mR_M_MeOH	R_M^0_Acet	*b*_Acet	*PC1*_Acet	C_0_Acet	*m*R_M_Acet	R_M^0_Diox	*b*_Diox	*PC1*_Diox	C_0_Diox	*m*R_M_Diox	R_{M}_*MLC1*	R_{M}_*MLC2*
1	1.25	-0.01	-3.65	95.06	0.07	1.16	-0.02	-4.96	73.22	-0.07	2.94	-0.04	-5.00	67.77	-0.31	0.37	0.12
2	2.90	-0.03	-2.79	94.64	0.14	3.55	-0.04	-2.08	80.22	0.12	3.39	-0.05	-0.98	72.79	-0.10	0.39	0.17
3	3.33	-0.03	0.33	100.60	0.35	3.18	-0.04	1.02	84.99	0.28	4.28	-0.06	1.59	75.69	0.04	0.44	0.23
4	3.75	-0.04	3.19	105.31	0.54	3.94	-0.05	2.71	85.93	0.39	5.19	-0.07	0.30	76.43	0.10	0.53	0.30
5	3.49	-0.03	0.76	101.07	0.38	3.61	-0.04	0.78	83.85	0.27	4.89	-0.06	1.71	75.63	0.04	0.57	0.34
6	3.79	-0.04	1.45	101.51	0.43	3.68	-0.04	0.23	83.10	0.25	4.95	-0.07	1.17	74.51	-0.03	0.57	0.34
7	3.68	-0.04	-0.13	98.75	0.33	4.09	-0.05	1.12	83.68	0.30	4.74	-0.06	0.86	75.35	0.02	0.57	0.37
8	2.65	-0.03	-1.72	97.71	0.21	2.69	-0.03	-1.67	81.33	0.13	4.34	-0.06	-1.10	72.43	-0.15	0.46	0.24
9	3.10	-0.03	-0.28	99.94	0.31	3.25	-0.04	0.37	83.72	0.24	4.05	-0.05	-0.07	73.96	-0.06	0.54	0.32
10	4.02	-0.04	1.76	101.45	0.45	4.09	-0.05	2.32	84.99	0.36	4.47	-0.06	1.04	75.70	0.04	0.62	0.37
11	3.74	-0.04	1.82	102.46	0.45	3.78	-0.04	2.22	85.33	0.35	4.50	-0.06	-1.88	75.22	0.01	0.53	0.30
12	3.85	-0.04	3.90	106.40	0.59	3.84	-0.05	1.76	84.67	0.32	5.16	-0.07	1.31	74.95	0.00	0.53	0.30
13	3.72	-0.04	-1.18	96.71	0.26	4.66	-0.06	0.72	82.68	0.29	5.49	-0.07	-0.77	73.52	-0.11	0.54	0.32
14	4.01	-0.04	2.24	102.41	0.49	4.07	-0.05	1.29	83.73	0.30	4.61	-0.06	-0.29	75.21	0.01	0.52	0.30
15	3.23	-0.03	-1.52	96.90	0.23	4.33	-0.05	-0.66	81.27	0.20	5.11	-0.07	-2.16	73.87	-0.08	0.49	0.32
16	2.57	-0.03	-1.50	98.56	0.22	2.94	-0.04	-3.17	78.68	0.04	3.36	-0.05	2.63	72.08	-0.14	0.37	0.19
17	2.58	-0.03	-2.68	95.36	0.15	2.92	-0.04	-2.02	80.43	0.11	3.54	-0.05	1.65	73.93	-0.05	0.35	0.17

Table S3. SRD scores for standardized (Std), range scaled (Rng) and Rank (Rnk) lipophilicity data.

Std		Rng		Rnk	
Variable	**SRD**	**Variable**	**SRD**	**Variable**	**SRD**
XlogP2	13.89	XlogP2	13.89	milogP	13.89
*PC1*_Acet	13.89	*PC1*_Acet	13.89	XlogP2	13.89
milogP	15.28	milogP	15.28	AlogP	15.97
mR_M_Acet	15.28	mR_M_Acet	15.28	XlogP3	16.67
AlogP	15.97	AlogP	15.97	*PC1*_Acetone	16.67
XlogP3	19.44	XlogP3	19.44	KOWWIN	18.06
R_M^0_MeOH	19.44	R_M^0_MeOH	19.44	mR_M_Acetone	18.06
mlogP	20.14	mlogP	20.14	R_M^0_MeOH	19.44
KOWWIN	20.83	KOWWIN	20.83	mlogP	20.14
AClogP	20.83	AClogP	20.83	AClogP	20.83
AlogpS	20.83	AlogpS	20.83	AlogpS	22.22
AlogPs	23.61	AlogPs	23.61	mR_M_MeOH	22.22
*b*_MeOH	23.61	*b*_MeOH	23.61	*b*_MeOH	23.61
mR_M_MeOH	23.61	mR_M_MeOH	23.61	*PC1*_MeOH	23.61
C_0_Acet	23.61	C_0_Acet	23.61	AlogPs	25.00
C_0_Diox	23.61	C_0_Diox	23.61	C_0_Acet	26.39
*PC1*_MeOH	25.00	*PC1*_MeOH	25.00	C_0_Diox	26.39
mR_M_Diox	25.00	mR_M_Diox	25.00	mR_M_Diox	26.39
R_M^0_Diox	26.39	R_M^0_Diox	26.39	R_M^0_Diox	27.78
C_0_MeOH	31.94	C_0_MeOH	31.94	C_0_MeOH	30.56
R_M^0_Acet	31.94	R_M^0_Acet	31.94	R_M^0_Acet	31.94
*b*_Diox	33.33	b_Diox	33.33	*b*_Diox	31.94
R_M_MELC1	33.33	R_M_MELC1	33.33	R_M_MELC1	31.94
*b*_Acet	34.72	*b*_Acet	34.72	R_M_MELC2	34.03
R_M_MELC2	36.11	R_M_MELC2	36.11	*b*_Acet	34.72
*PC1*_Diox	59.72	*PC1*_Diox	59.72	*PC1*_Diox	59.72

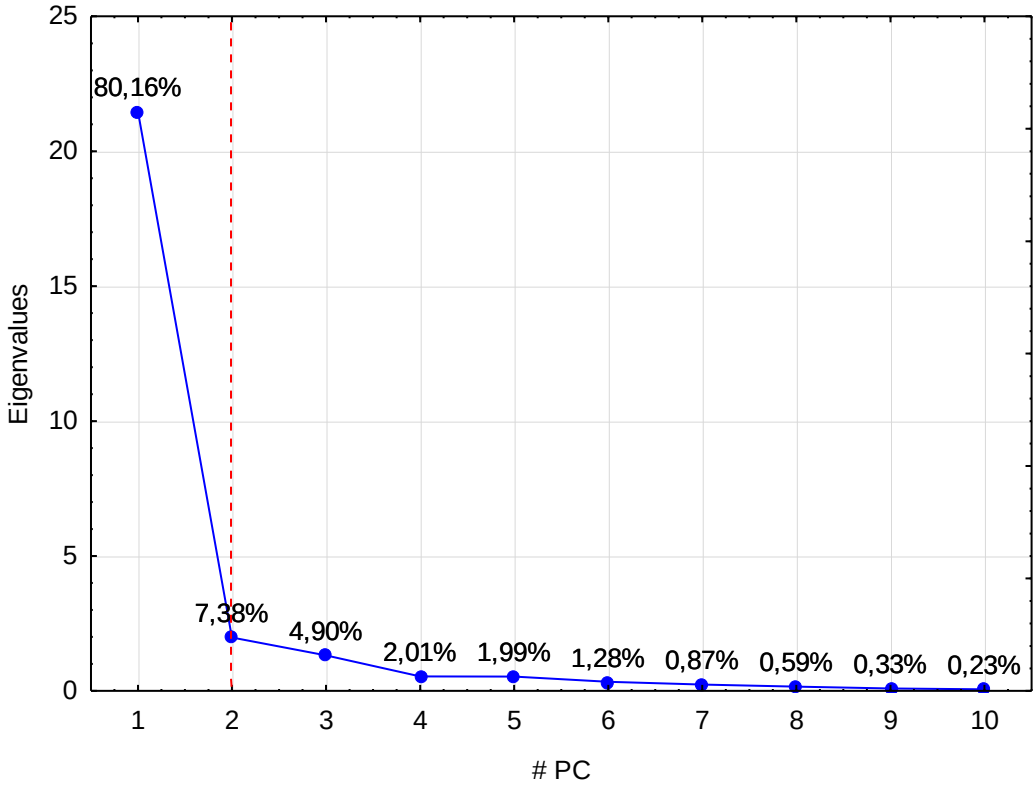

Figure S1 Eigenvalues scree plot showing distribution of data variability by principal components. Following the "broken stick" rule the first two principal components can be selected to efficiently describe retention data structure.

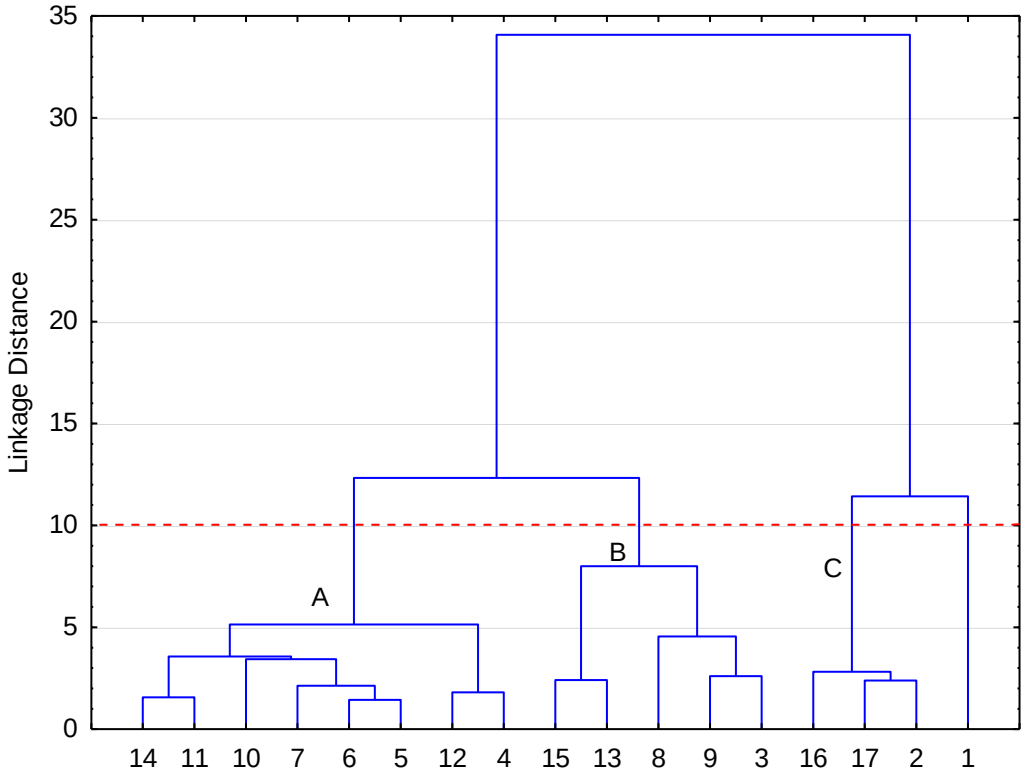

Figure S2 HCA of retention data of compounds. Three clusters (A, B and C) can be observed at linkage distance of 10 units and one outlier (compound no. 1). For numeration and chemical structures of compounds see Table 1 in the manuscript