Supporting Information

In silico Comparison of Antimycobacterial Natural Products with Known Antituberculosis Drugs

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A. Cluster number and physicochemical properties of natural products.

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
9-Methyladenine	1	149.15	-0.37	0	4	1	0
Agelasine E	1	422.63	4.89	8	3	1	0
Micromolide	2	280.45	5.99	12	1	0	2
Panamycin-607	2	621.89	6.36	9	6	0	2
3-Epi-astrahygrol	2	442.67	6.74	2	2	1	1

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Pyrrolnitrin	3	257.07	3.56	2	2	1	0
Cyanthiwigin C	4	302.45	3.91	1	2	1	0
Manoalide 25-acetate	4	458.59	6.56	9	4	1	1
*NPMC3	4	260.37	5.78	8	2	2	1
Lincomolide B	4	278.39	2.89	9	2	1	0
*NPMC18c	4	382.49	6.7	9	3	2	1
Lecheronol A	4	306.44	2.95	0	3	2	0
Imberbic acid	4	458.67	5.72	1	4	3	1
α-Humulene	4	204.35	6.1	0	0	0	1
*EJMC51	4	296.53	8.05	13	1	1	2
(E)-Phytol	4	290.48	7.84	10	1	1	1
Scytoscalarol	4	415.66	4.99	3	2	4	0
Oleanolic acid	4	456.7	6.88	1	3	2	1
*EJMC67	4	530.74	6.59	7	4	1	2
Squalene	4	410.72	9	15	0	0	2
Tetrahydroxysqualene	4	474.72	7.99	19	4	4	2
Globiferin	4	242.31	4.5	0	2	0	0
Litseakolide L	4	340.5	4.83	13	3	1	1
Oplopandiol	4	262.39	5.47	8	2	2	1
Falcarindiol	4	260.37	5.78	8	2	2	1
Elisapterosin B	5	314.42	4.53	1	2	1	0
7-Methyljuglon	5	188.18	1.58	0	3	1	0
*NPMC20c	5	364.31	0.99	0	7	1	0
*NPMC20d	5	366.32	1.21	0	7	1	0
*NPMC20e	5	396.35	0.66	1	8	1	0
*NPMC20g	5	332.31	3.81	0	5	1	0
Usnic acid	5	344.32	0.66	2	6	3	0
Phomoxanthone B	5	750.7	4.26	11	10	4	2
*NPMC31c	5	337.5	6.55	10	1	0	1
*NPMC31d	5	365.55	7.53	12	1	0	2
*NPMC40	5	372.5	4.64	6	3	1	0
Phomoxanthone A	5	750.7	4.19	11	10	4	2
*NPMC22b	5	582.55	1.31	3	10	8	2
Khonklonginol A	5	436.5	5.1	4	6	2	1
Khonklonginol B	5	436.5	5.1	4	6	2	1
Khonklonginol H	5	436.5	5.94	4	6	2	1
Lupinifolinol	5	422.47	4.61	3	6	3	0
Dehydrolupinifolinol	5	420.45	5.98	3	6	3	1

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Flemichin	5	422.47	5.45	3	6	3	1
Eriosemaone A	5	422.47	5.45	3	6	3	1
Lupinifolin	5	406.47	5.77	3	5	2	1
*EJMC146	5	484.45	3.72	6	8	2	0
Karanjachromene	5	334.37	4.89	2	4	0	0
Isobavachalcone	5	324.37	4.7	5	4	3	0
*EJMC158	5	406.47	6.08	5	5	3	1
*EJMC159	5	324.37	4.69	5	4	3	0
*EJMC171	5	562.61	6.42	18	6	1	3
α-Mangostin	5	408.49	6.68	5	5	3	1
Mollicellin K	5	382.36	5.22	3	6	2	1
*EJMC185	5	466.39	1.51	4	9	4	0
*EJMC187	5	262.26	1.62	3	5	1	0
*EJMC188	5	320.29	1.17	5	6	1	0
2-Methoxyjuglone	5	204.18	0.91	1	4	1	0
3-Methoxyjuglone	5	204.18	0.91	1	4	1	0
*EJMC197	5	1258.02	9	45	6	0	3
Perforamone B	5	290.31	2.59	4	5	2	0
Perforamone D	5	274.27	1.5	1	5	2	0
Peucin-7-methyl ether	5	274.31	3.83	3	4	1	0
Greveichromenol	5	274.27	1.57	1	5	2	0
Myxopyronin A	5	417.5	5.14	12	4	2	2
Phomoenamide	6	284.35	1.25	9	4	4	0
Cis-pentacin	6	129.16	0.04	1	3	2	0
Cryptolepine	7	233.29	0.56	0	0	1	0
Ingenamine G	8	464.73	7.15	0	3	1	1
Neopetrosiamine A	8	440.75	8.62	0	2	0	1
Halicyclamine A	8	462.75	9	0	2	0	1
Cyclostelletamine A	9	492.82	3.49	0	0	0	0
Cyclostelletamine B	9	506.85	2.71	0	0	0	1
Cyclostelletamine C	9	520.88	3.2	0	0	0	1
Cyclostelletamine D	9	520.88	3.2	0	0	0	1
Cyclostelletamine E	9	534.9	3.69	0	0	0	1
Cyclostelletamine F	9	548.93	4.18	0	0	0	1
3-Nitropropionic acid	10	119.08	-0.63	3	4	1	0
Linoleic acid	10	280.45	6.66	14	2	1	2
Exocarpic acid	10	274.4	5.98	10	2	1	1
*EJMC222	10	286.41	7.02	10	2	1	1

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Antihelminthicin A	10	266.38	4.43	11	3	1	1
Chaulmoogric acid	10	280.45	6.73	13	2	1	2
Monamphilectine A	11	423.63	3.55	6	2	0	0
8,15-Diisocyano-11(20)-amphilectene	11	324.5	1.27	2	0	0	0
*Marine45	12	682.27	0.04	7	10	8	2
*Marine46	12	491.13	0.47	6	6	4	0
*NPMC7a	12	360.53	7.35	16	3	1	2
*NPMC8a	12	410.67	9	19	1	0	2
*NPMC34b	12	220.23	2.05	0	2	0	0
*NPMC34c	12	236.23	1.73	0	3	1	0
Manzamine E	12	564.76	5.45	1	5	2	2
Hydroxymanzamine E	12	580.76	5.03	1	6	3	2
Ascididemin	12	283.28	3.31	0	4	0	0
Diplamine	12	363.43	2.21	5	4	1	0
Isodiplamine	12	363.43	2.57	5	4	1	0
Shermilamine B	12	390.46	1.62	4	3	3	0
11-Hydroascididemin	12	299.28	2.85	0	5	1	0
Kuanoniamine A	12	289.31	3.18	0	4	0	0
(-)-8-Hydroxymanzamine A	12	564.76	6.45	1	5	3	2
(-)-Manzamine F	12	580.76	4.63	1	6	3	1
Manzamine A	12	548.76	7.27	1	4	2	2
(+)-8-Hydroxymanzamine A	12	564.76	6.45	1	5	3	2
*EJMC235	12	370.57	8.88	16	2	1	2
*EJMC236	12	374.56	7.94	17	2	0	2
3-Methoxycarboxy-1,5-Dihydroxyantraquinone	13	298.25	2.49	2	5	2	0
(+)-Calanolide A	13	370.44	4.89	2	4	1	0
Ecteinascindin 770	13	766.84	2.04	4	12	3	2
Ecteinascindin 786	13	768.81	0.93	4	13	3	2
15-Acetoxyorbiculin	13	684.73	7.65	13	6	0	3
Salasol A	13	518.55	3.6	9	6	1	1
Celahin C	13	518.55	3.6	9	6	1	1
*EJMC4	13	642.69	6.93	11	6	1	3
*EJMC5	13	642.69	6.93	11	6	1	3
Mutangin	13	622.66	5.98	12	6	0	3

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Orbiculin G	13	640.72	8.32	11	5	0	3
Triptogelin G-2	13	428.56	6.19	5	3	0	1
*EJMC36	13	524.6	4.31	7	6	1	1
*EJMC48	13	678.77	6.05	10	7	3	2
*EJMC50	13	758.81	3.75	15	8	1	2
Epoxybeilschmin A	13	430.45	3.57	6	8	0	0
Epoxybeilschmin B	13	446.49	3.5	8	8	0	0
Beilschmin D	13	414.41	3.64	4	8	0	0
Beilschmin B	13	432.51	4.13	8	7	0	0
Feruloyltyramine	13	343.37	2.65	8	5	3	0
α-Mangostin-3-sulphate	13	488.55	4.5	7	7	3	0
*EJMC243	13	272.34	2.86	6	3	2	0
Methyl-7-methoxy anodendroate	13	266.29	2.41	4	4	1	0
Wutaiensal	13	262.3	2.31	4	4	1	0
*EJMC237	14	898.34	9	45	10	8	3
*EJMC238	14	911.04	1.04	10	18	8	3
*EJMC239	14	939.09	1.72	11	18	8	4
*EJMC240	14	1073.22	1.7	31	22	11	4
*EJMC241	14	1055.2	2.88	30	21	10	4
Batzelladine L	15	653	8.35	19	3	2	3
Batzelladine N	15	622.93	7.4	17	3	2	3
Crambescidine 800	15	799.18	8.87	27	7	4	3
Pellitorine	15	223.35	4.45	9	1	1	0
*EJMC225	15	332.43	5.8	12	3	2	2
Antihelminthicin B	15	298.42	3.99	13	3	2	1
Antihelminthicin C	15	354.52	5.96	17	3	2	2
Ethyl chaulmoograte	15	308.5	7.78	15	1	0	2
Debilisone C	15	386.57	7.03	14	2	1	2
Debilisone E	15	384.55	6.61	14	2	1	2
Trichoderin A	15	1162.59	5.18	39	13	10	5
Pulpularin A	15	775.93	3.84	10	8	3	1
Pulpularin C	15	761.9	3.35	9	8	3	1
12-Deacetoxyscalarin-19-acetate	17	428.6	5.99	2	2	0	1
*NPMC39	17	386.48	4.06	4	4	0	0
Protoprimulagenin A	17	458.72	6.01	0	3	2	1
*NPMC54a	17	695.11	9	22	1	0	3

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Suberosol B	17	236.35	3.49	0	2	1	0
Azorellanone	17	304.47	3.68	1	2	1	0
Azorellanol	17	348.52	4.77	3	2	1	0
17-Acetoxy-13α-hydroxyazorellane	17	362.55	4.9	4	2	1	0
*EJMC27	17	376.53	4.58	5	3	0	0
9α,13α-Epidioxyabiet-8(14)-en-18-oic acid	17	334.45	4.22	2	2	1	0
Horminone	17	332.43	2.77	1	3	2	0
Ent-3β-hydroxytrachylobane	17	288.47	4.34	0	1	1	0
Ent-3β-hydroxytrachyloban-2-one	17	286.45	3.96	0	1	0	0
Ent-3β-acetoxy-19-hydroxytrachylobane	17	346.5	3.86	3	2	1	0
Ent-trachyloban-17-al	17	286.45	4.45	1	0	0	0
Kaurenoic acid	17	302.45	4.79	1	2	1	0
Escobarine A	17	314.42	4.05	1	3	0	0
Escobarine B	17	316.43	3.17	1	3	1	0
*EJMC56	17	476.73	4.73	2	4	4	0
Bonianic acid A	17	484.71	7.57	7	3	1	1
Bonianic acid B	17	500.71	5.85	8	4	1	2
3-Epi-astrapteridiol	17	444.69	7.22	2	3	2	1
Aegicerin	17	442.67	5.33	0	3	1	1
α-Tocospiro A	17	460.73	7.73	13	3	1	2
(-)-4-Hydroxy-1-tetralone	18	162.19	1.37	0	2	1	0
*NPMC47a	18	674.91	9	8	5	1	2
*NPMC47b	18	632.87	9	6	5	2	2
*EJMC133	18	325.4	4.42	7	3	0	0
*EJMC168	18	194.18	1.86	3	3	2	0
*EJMC169	18	206.24	2.98	5	2	0	0
(+)-Altholactone	18	232.23	0.31	1	3	1	0
Howiinin A	18	362.38	2.7	6	3	0	0
Ripostatin A	18	494.62	5.91	9	5	2	1
Sarmentine	19	221.34	3.87	7	1	0	0
α-Tocospiro B	19	448.68	7.3	13	4	1	2
α-Tocopherylquinone	19	446.71	9	15	3	1	2
*EJMC214	19	392.57	8.57	15	1	0	2

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Plakortolide J	19	390.56	7.49	12	1	0	2
*EJMC217	19	368.59	7.57	15	2	1	2
*EJMC218	19	398.62	6.79	17	3	2	2
*EJMC220	19	290.4	4.92	10	3	2	0
*EJMC221	19	348.48	5.21	14	3	2	1
Ambiguine K	20	420.97	2.55	1	1	2	0
Ambiguine L	20	386.53	2.33	1	1	2	0
Ambiguine M	20	438.99	0.92	1	2	3	0
Ambiguine N	20	404.54	0.69	1	2	3	0
Ambiguine A isonitrile	20	406.99	3.96	3	0	1	0
Ambiguine C isonitrile	20	388.55	2.51	3	1	2	0
Ambiguine E isonitrile	20	436.97	0.79	1	2	2	0
Ambiguine I isonitrile	20	402.53	0.57	1	2	2	0
Hapalindole G	20	338.87	2.12	1	0	1	0
Hapalindole H	20	304.43	1.89	1	0	1	0
Fischambiguine B	20	436.97	2.95	1	3	2	0
Ambiguine G nitrile	20	402.96	5.45	1	1	1	1
Diaportheine B	21	364.43	0.21	1	6	4	0
Diaportheine A	21	366.45	-0.18	1	6	5	0
Trichoderin A1	21	1144.57	7.43	46	12	9	5
Trichoderin B	21	1148.56	5.85	46	13	10	5
Calpinactam	21	767.91	0.84	26	10	9	3
*NPMC4a	22	363.35	5.69	11	1	0	2
*NPMC4b	22	360.53	4.23	13	2	0	1
Ugandensidial	22	308.37	0.85	4	4	1	0
*EJMC19	22	262.3	2.11	1	3	1	0
Batzelladine M	22	594.87	6.61	16	3	2	3
Batzelladine C	22	488.71	4.9	18	3	4	1
Hymenidin	23	348.63	-0.18	5	3	5	0
Monobromoisophakellin	23	308.18	0.23	0	2	3	0
*EJMC127	24	173.26	0.58	2	1	0	0
Isogoyazensolide	26	360.36	0.97	3	5	1	0
Isocentratherin	26	374.38	1.36	3	5	1	0
5-Epi-isogoyazensolide	26	360.36	0.97	3	5	1	0
* 5-Epi-isocentratherin	26	374.38	1.36	3	5	1	0
*EJMC37	26	529.02	4.99	6	5	1	1
Kuanoniamine D	26	363.48	1.43	4	4	1	0
(-)-Atrop-abyssomicin C	26	348.39	-0.14	0	5	2	0

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Borrelidin	26	489.64	3.58	2	6	3	0
Mupirocin	26	500.62	3.99	17	8	4	2
Thuggacin A	26	631.86	5.65	11	7	5	3
*NPMC20a	28	364.31	2.33	0	7	2	0
Banegasine	28	204.23	0.92	2	4	3	0
Ramiferin	28	492.65	7.62	0	5	3	1
15-Hydroxydehydroabietic acid	28	316.43	3.45	2	3	2	0
*EJMC160	28	340.37	3.49	3	5	3	0
*EJMC180	28	378.37	-0.02	4	8	5	0
*EJMC182	28	458.41	1.04	5	9	4	0
*EJMC183	28	208.21	0.36	1	4	2	0
Plakortolide F	28	390.51	5.84	10	2	1	1
Debilisone B	28	404.58	6.34	15	3	2	2
Pitiprolamide	28	905.13	4.69	7	8	2	1
Sansanmycin A	28	863.94	0.17	23	12	10	4
Sansanmycin F	28	904	1.98	21	12	10	4
Sansanmycin G	28	885.96	2.62	20	12	10	4
Cordycommunin	28	860.05	2.43	15	10	9	3
*NPMC33d	29	414.61	5.83	9	2	1	1
Agelasine D	29	436.66	4.31	5	3	1	0
*NPMC33e	29	426.62	6.12	7	2	1	1
*NPMC33f	29	468.7	6.37	6	2	1	1
*NPMC33g	29	510.78	7.54	7	2	1	2
Azadiradione	29	450.57	4.11	3	4	0	0
Epoxyazadiradione	29	466.57	3.96	3	5	0	0
Cordiachrome B	29	242.31	3.66	0	2	0	0
Goyazensolide	30	360.36	0.59	4	5	1	0
Centratherin	30	374.38	0.97	4	5	1	0
Lychnophorolide B	30	374.38	0.97	4	5	1	0
Corallolide B	30	360.4	0.92	1	5	2	0
Bipinnapterolide B	30	360.4	3.16	2	5	0	0
*EJMC28	30	390.56	5.07	6	3	0	1
Caniojane	30	356.46	5.56	1	2	0	1
Chaetoviridine E	30	414.88	4.95	5	4	0	0
Cordiachrome C	30	242.31	3.85	2	2	0	0
4-Methoxy-2-phenylquinoline	31	235.28	4.14	2	2	0	0

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Graveolinine	31	279.29	4.01	2	4	0	0
Kokusagine	31	243.21	2.59	1	5	0	0
Dictamnine	31	199.21	2.8	1	3	0	0
γ-Fagarine	31	229.23	2.67	2	4	0	0
Bidebiline E	31	584.62	6.98	3	6	2	2
Liriodenine	31	275.26	3.62	0	4	0	0
Oxostephanine	31	305.28	3.36	1	5	0	0
(-)-Nordicentrine	31	325.36	2.75	2	5	1	0
Lacheolatin B	31	262.26	4.38	1	3	0	0
Linosterol	32	414.66	7.44	6	2	2	1
Nephalsterol B	32	430.66	5.82	6	3	3	1
Nephalsterol C	32	472.7	6.55	8	3	2	1
Axisonitrile-3	32	231.38	4.41	1	1	0	0
Saringosterol	32	428.69	7.36	6	2	2	1
*NPMC41	32	388.54	5.91	7	2	0	1
*NPMC54b	32	428.65	6.35	4	1	1	1
6-Hydroxyculactone	32	482.69	5.02	3	3	1	1
*NPMC51	32	410.72	9	5	0	0	1
*NPMC52	32	408.7	9	5	0	0	1
*NPMC53	32	444.69	7.54	5	1	1	1
*NPMC54c	32	442.67	6.84	5	1	1	1
*NPMC54d	32	428.69	6.99	6	2	1	1
*NPMC55a	32	414.66	7.72	6	2	1	1
*NPMC55b	32	428.69	8.21	7	2	1	1
Mulinol	32	334.54	5.16	2	2	2	1
*EJMC26	32	362.55	5.87	5	2	1	1
Pimaric acid	32	302.45	4.68	2	2	1	0
*EJMC39	32	316.48	6.67	6	1	0	1
Ursolic acid	32	456.7	6.89	1	3	2	1
Betulinic acid	32	456.7	7	2	3	2	1
*EJMC68	32	458.72	6.7	6	1	1	1
*EJMC69	32	458.72	6.27	5	1	1	1
Ergosterol peroxide	32	428.65	6.35	4	1	1	1
β-Sitostenone	32	410.67	8.5	6	1	0	1
*EJMC74	32	412.6	6.84	4	1	1	1
*EJMC75	32	426.63	7.03	4	1	1	1
Parguesterol A	32	412.65	7.59	6	2	1	1
Parguesterol B	32	430.66	6.66	6	3	2	1

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Pseudopyronine A	33	266.38	4.95	9	2	1	0
Pseudopyronine B	33	294.43	5.93	11	2	1	2
6,7-Dehydroroyleanone	33	314.42	4.38	1	2	1	0
7α-Acetoxy, 6β-hydroxyroyleanone	33	390.47	2.51	3	4	2	0
Callicarpic acid B	33	330.42	4.2	5	4	1	0
Thiolactomycin	33	210.29	3.46	2	0	1	0
*NPMC20h	34	334.32	3.33	0	5	2	0
*NPMC31a	34	311.46	5.95	9	1	0	1
*NPMC31b	34	339.51	6.93	11	1	0	2
Manadomanzamines A	34	610.87	5.29	2	5	3	2
Manadomanzamines B	34	610.87	5.29	2	5	3	2
Desacetyl-pyramidaglain D	34	652.73	4.08	14	8	4	2
Pseudopteroxazole	35	309.45	6.38	1	1	0	1
Homopseudopteroxazole	35	379.58	8.61	5	1	0	1
Seco-pseudopteroxazole	35	311.46	7.04	4	1	0	1
Erogorgiaene	35	270.45	7.42	4	0	0	1
7-Hydroxy-erogorgiaene	35	286.45	7.1	4	1	1	1
Ostruthin	35	298.38	5.7	5	2	1	1
*EJMC49	35	698.75	5.38	13	7	0	3
Brachystamide B	35	411.58	7.95	15	3	1	2
Elaeagin	35	258.31	3.19	4	3	1	0
Cordiachromene	35	230.3	4.51	3	2	1	0
*Marine47	36	522.23	2.05	14	5	5	2
*Marine48	36	518.2	2.14	11	6	4	2
Celastramycin B	36	372.76	2.67	0	6	3	0
Celastramycin A	36	390.69	5.5	7	3	3	1
Carnosic acid	36	332.43	4.07	2	4	3	0
Malabaricone A	36	326.43	5.78	10	3	2	1
Dodecanoyl-phloroglucinol	36	308.41	5.45	11	4	3	2
Ochratoxin A	36	403.81	3.72	6	5	3	0
(+)-Araguspongine	37	478.71	5.84	0	6	2	1
(-)-Araguspongine C	37	478.71	5.84	0	6	2	1
Enniatins H	38	653.85	2.77	7	6	0	1
Enniatins I	38	667.87	3.26	8	6	0	1
Enniatins B	38	639.82	2.28	6	6	0	1

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Enniatins B4	38	653.85	2.77	7	6	0	1
Elisabethin A	39	316.43	3.71	1	2	1	0
Colombiasin A	39	314.42	2.99	0	2	1	0
Cumbiasin A	39	332.43	3.35	1	4	2	0
Cumbiasin B	39	348.43	2.94	1	5	3	0
6β,7α-Dihydroxyroyleanone	39	348.43	1.77	1	4	3	0
Elisabethin H	39	252.31	1.82	2	3	2	0
(-)-Abyssomicin C	39	346.37	0.12	0	5	1	0
Engelhardion	40	312.36	4.56	0	4	2	0
Ferulenol	40	366.49	8.13	8	2	1	1
*NPMC18b	40	486.6	9	12	3	1	2
*NPMC18d	40	424.53	7.72	11	3	1	2
Sarmentosine	40	299.36	3.58	6	3	0	0
Brachyamide B	40	327.42	4.56	8	3	0	0
*EJMC147	40	324.28	3.93	1	6	0	0
Demethoxykanugin	40	326.3	3.64	3	6	0	0
3,7-Dimethoxyflavone	40	282.29	3.77	3	4	0	0
Maackiain	40	284.26	2.71	0	5	1	0
Pinnatin	40	296.27	3.43	2	5	0	0
Pinocembrine	40	256.25	2.46	1	4	2	0
Dalparvone	40	330.29	2.03	3	7	3	0
Beilschmin A	40	416.46	4.2	6	7	0	0
Dalparvinene	40	286.32	3.47	5	4	2	0
Demethoxycurcumin	40	338.35	3.86	6	4	3	0
Ehretiquinone	40	348.39	4.16	2	4	1	0
*EJMC184	40	224.21	0	1	5	3	0
Naphthalenone	40	194.18	0.51	0	4	3	0
Eucapsitrione	40	358.3	3.45	0	6	3	0
Engelharquinone	40	348.31	0.93	0	6	3	0
Diffractaic acid	40	374.38	4.24	6	6	2	0
Alliodorin	40	260.33	3.71	6	3	2	0
7-Hydroxymukonal	41	241.24	3.04	2	3	2	0
Scopoletin	41	192.17	1.24	1	3	1	0
*EJMC175	41	662.68	6.01	9	10	2	2
*EJMC176	41	662.68	5.81	9	10	2	2
Rumexneposide A	41	446.45	1.59	7	8	4	0
Torachrysone	41	246.26	2.59	2	4	2	0

Compound	Cluster Number	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
*EJMC181	41	408.4	0.07	5	9	5	0
7-Methoxy wutaifuranal	41	202.21	2.48	3	3	0	0
Ecteinascidin 743	42	761.84	1.82	4	12	4	2
Lissoclinidine	42	364.46	4.67	4	3	1	0
Corallopyronin A	42	527.65	6.59	16	5	3	3
Massetolide A	43	1140.41	3.28	31	15	13	4
Viscosin	43	1126.38	2.79	30	15	13	4
Syringomycin E	43	1225.78	-4.97	28	19	19	4
Lydiamycin A	43	663.76	-0.61	13	9	5	2
Brunsvicamide B	43	859.07	6.37	15	8	8	4
Brunsvicamide C	43	877.04	4.41	17	10	8	3
Dehydrobatzelladine C	43	486.69	6.1	18	4	3	2
*Marine49a	44	733.04	2.93	10	7	3	1
*Marine49b	44	749.04	1.77	10	8	4	1
Nocathiacin	44	1436.51	0.13	10	21	9	3
Nocardithiocin	44	1161.36	6.4	12	17	8	5
Kahalalide A	45	880.04	1.79	16	10	9	3
*NPMC10	45	248.32	3.5	5	2	0	0
*NPMC11	45	246.3	3.55	4	2	0	0
Pyrone	45	274.27	2.79	4	4	0	0
*NPMC20b	45	368.34	2.05	0	7	2	0
*NPMC20f	45	382.32	0.21	0	8	2	0
Hirsutellone A	45	445.55	5.07	1	4	1	1
Hirsutellone B	45	459.58	5.45	1	4	1	1
Hirsutellone C	45	447.57	4.63	1	4	2	0
Hirsutellone D	45	461.55	4.46	1	5	2	0
Hirsutellone F	45	891.1	9	3	8	2	2
Bauhinoxepin J	45	256.25	2.68	1	4	0	0
Erythrophloin C	45	404.58	7.62	10	1	0	1

*Generic name assigned to differentiate unnamed compounds reported in literature reference[1]

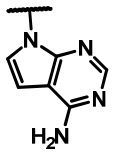
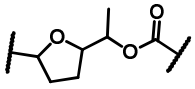
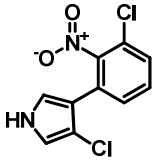
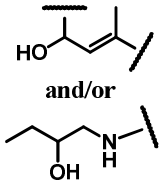
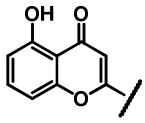
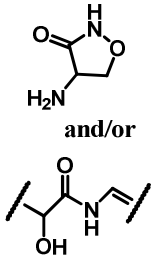
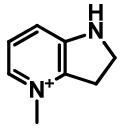
B. Cluster number and physicochemical properties of conventional antituberculosis drugs.

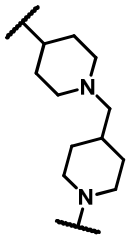
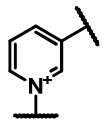
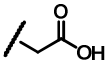
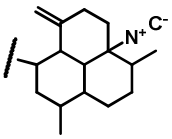
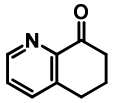
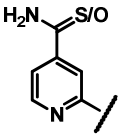
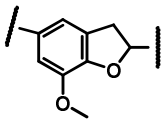
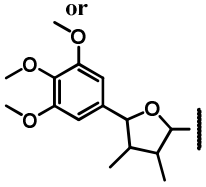
Compound	Cluster Group	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
Clarithromycin	2	747.95	2.33	8	4	13	2
Ethambutol	4	204.31	-0.38	9	4	4	0
Terizidone	6	302.29	-1.07	4	2	4	0
Cycloserine	6	102.09	-2.08	0	2	2	0
Isoniazid	12	137.14	-1.01	2	2	2	0
Pyrazinamide	12	123.11	-1.03	1	1	3	0
Ethionamide	12	166.24	1.26	2	0	2	0
Prothionamide	12	180.27	1.75	3	0	2	0
Streptomycin	14	581.57	-6.72	9	12	14	3
Amikacin	14	585.60	-9.00	11	13	17	4
Kanamycin	14	484.50	-7.85	6	11	15	2
Capreomycin	16	668.71	-8.70	12	14	14	4
Linezolid	23	337.35	1.14	5	1	3	0
Clofazimine	25	473.40	6.98	4	1	2	3
Moxifloxacin	28	401.43	2.44	4	2	5	0
Ofloxacin	28	361.37	1.85	2	1	5	0
Thioacetazone	28	236.29	1.19	5	3	3	0
p-Aminosalicylic acid	28	153.14	0.67	1	3	4	0
Imipenem	28	299.35	-0.81	7	4	5	0
Amoxicillin	28	365.40	0.42	5	4	6	1
Clavulanate	28	199.16	-1.20	2	2	5	0
Levofloxacin	34	361.37	1.85	2	1	5	0
Rifampicin	42	822.94	4.57	5	6	13	2
Rifabutin	42	847.00	6.31	5	5	13	3
Cilastatin	43	358.45	-0.07	12	4	6	2

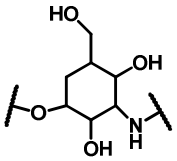
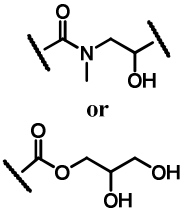
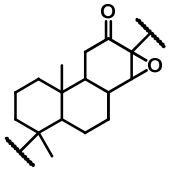
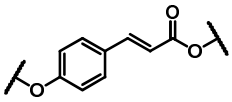
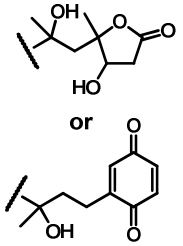
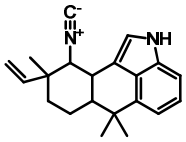
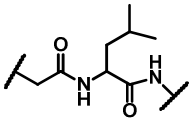
C. Cluster number and physicochemical properties of pre-clinical and clinical development compounds.

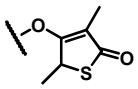
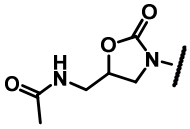
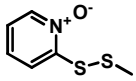
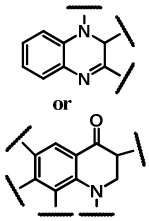
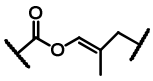
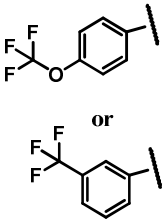
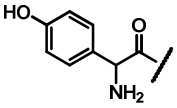
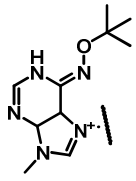
Compound	Cluster Group	Mwt	cLogP	Rot. Bonds	HBA	HBD	RO5 Dev
SQ109	4	330.55	5.52	9	2	2	1
SQ609	8	346.55	3.54	4	3	1	0
PNU-100480 (Sutezolid)	23	353.41	2.01	5	2	1	0
DC-159a	25	419.42	2.80	4	5	2	0
BTZ043	27	431.39	3.58	3	6	1	1
PA-824	27	359.26	2.86	6	6	0	1
OPC-67683	27	534.48	6.52	9	7	0	3
Sudoterb (LL3858)	27	519.56	4.91	8	3	1	1
Gatifloxacin	28	375.39	2.15	4	5	2	0
TMC207 (Bedaquiline)	34	555.50	7.70	8	4	1	2
Rifapentine	42	877.03	6.02	6	13	6	4
CPZEN-45	42	688.73	-2.75	12	13	7	4
SQ-641	43	751.82	0.38	20	12	6	4

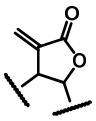
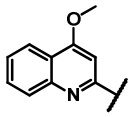
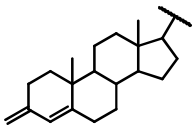
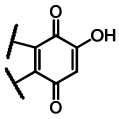
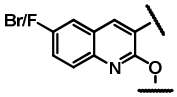
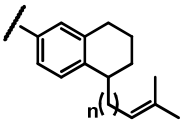
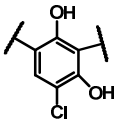
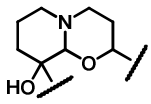
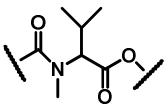
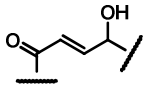
D. Cluster analysis results.

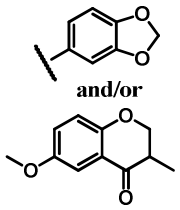
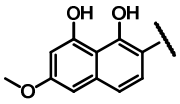
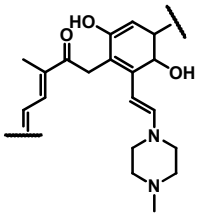
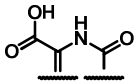
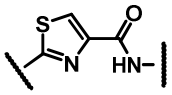
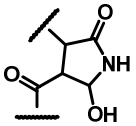
Cluster	Example of common functional group	CDs and/or DCs in cluster	Cluster size	Number of NPs
1		-	2	2
2		Clarithromycin	4	3
3		-	1	1
4		Ethambutol, SQ109	21	19
5		-	40	40
6		Terizidone, Cycloserine	4	2
7		-	1	1

Cluster	Example of common functional group	CDs and/or DCs in cluster	Cluster size	Number of NPs
8		SQ609	3	3
9		-	6	6
10		-	6	6
11		-	2	2
12	 **and/or** 	Prothionamide, Isoniazid, Pyrazinamide, Ethionamide	24	20
13	 **or** 	-	24	24

Cluster	Example of common functional group	CDs and/or DCs in cluster	Cluster size	Number of NPs
14		Streptomycin, Kanamycin, Amikacin	8	5
15		-	13	13
16	-	Capreomycin	1	0
17		-	24	24
18		-	9	9
19		-	9	9
20		-	12	12
21		-	5	5

Cluster	Example of common functional group	CDs and/or DCs in cluster	Cluster size	Number of NPs
22		-	6	6
23		Linezolid, PNU-100480 (Sutezolid)	4	2
24		-	1	1
25		DC-159a, Clofazimine	2	0
26		-	10	10
27		PA824, OPC67683, Sudoterb (LL3858), BTZ043	4	0
28		Amoxicillin, Clavulanate, Moxifloxacin, Ofloxacin, Thioacetazone, Imipenem, *p*-Aminosalicylic acid, Gatifloxacin	23	15
29		-	8	8

Cluster	Example of common functional group	CDs and/or DCs in cluster	Cluster size	Number of NPs
30		-	9	9
31		-	10	10
32		-	29	29
33		-	6	6
34		Levofloxacin, Ofloxacin, TMC207 (Bedaquiline)	8	6
35		-	10	10
36		-	8	8
37		-	2	2
38		-	4	4
39		-	7	7

Cluster	Example of common functional group	CDs and/or DCs in cluster	Cluster size	Number of NPs
40		-	23	23
41		-	8	8
42		Rifapentine, Rifampicin, Rifabutin, CPZEN-45	7	3
43		Cilastatine, SQ-641	9	7
44		-	4	4
45		-	13	13

E. References.

(1) (a) García, A., Bocanegra-García, V., Palma-Nicolás, J. P., Rivera, G. Vennerstrom, J. L. Recent Advances in Antitubercular Natural Products. *Eur. J. Med. Chem*. **2012**, *49*, 1-23. (b) Rogoza, L. N.; Salakhutdinov, N. F.; Tolstikov, G. A. Anti-tubercular Activity of Natural Products: Recent Developments. In *Opportunity, Challenge and Scope of Natural Products in Medicinal Chemistry*; Tiwari, V. K. Ed.; Research Signpost: India, 2011; pp 103-120. (c) De Souza, M. V. N, Marine Natural Products Against Tuberculosis. *The Scientific World Journal* **2006**, *6*, 847-861.