

Supporting Information

What Do Medicinal Chemists Actually Make? A 50-Year Retrospective

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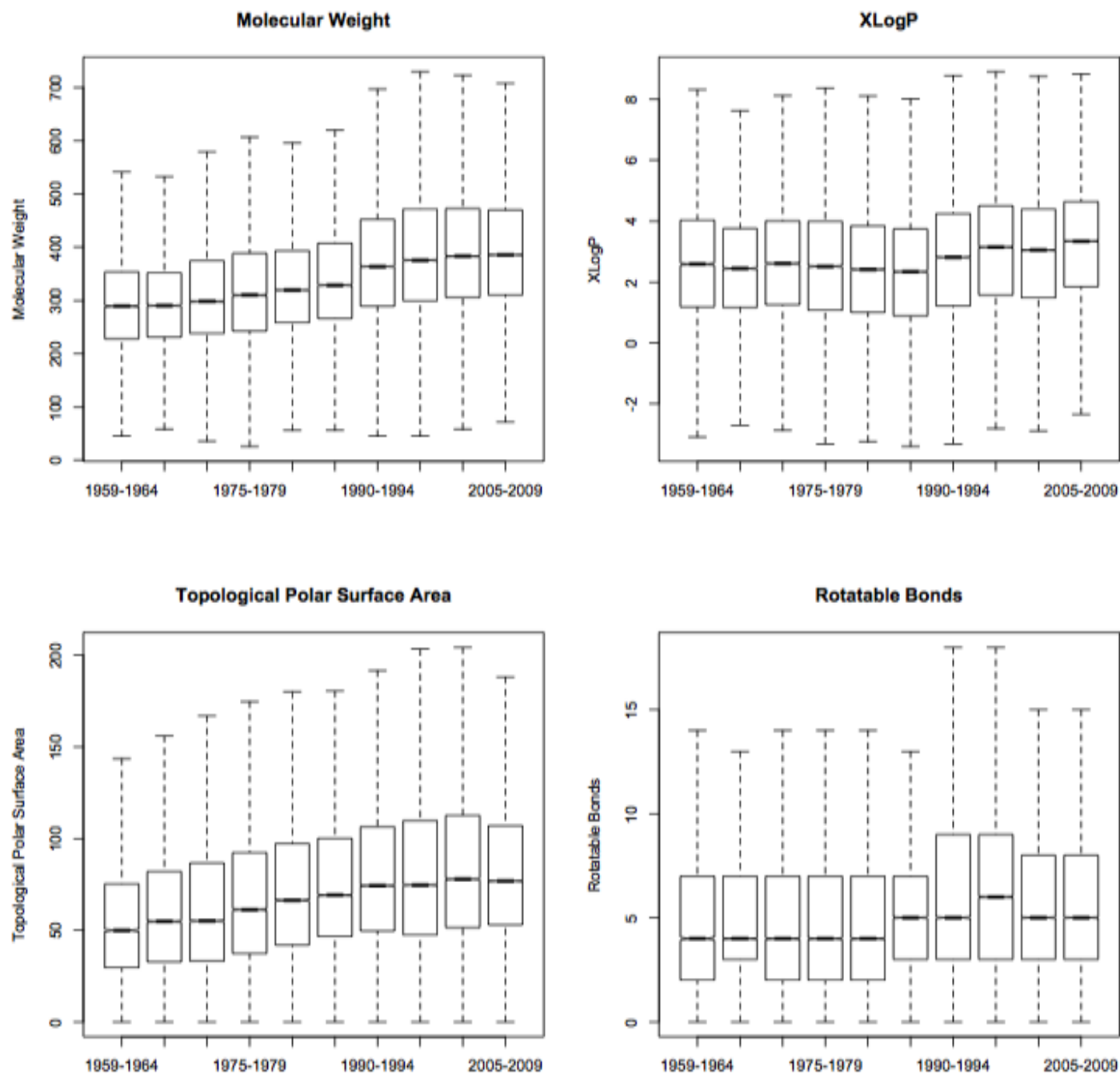
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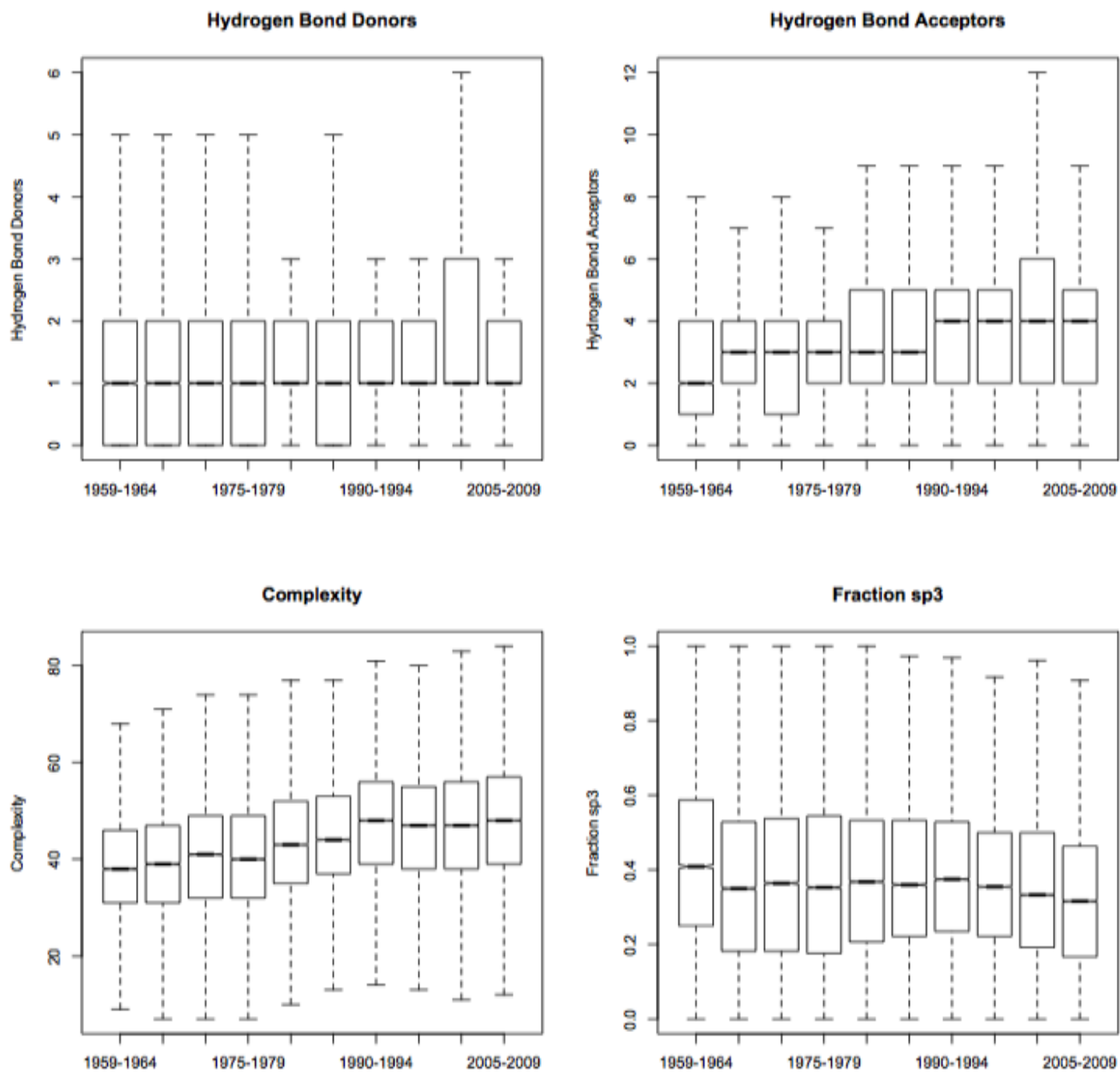
S2 - Box plots of molecular weight, calculated logP, topological polar surface area, and rotatable bonds for molecules appearing in JMC 1959-2009.

S3 - Box plots of number of hydrogen bond donors, number of hydrogen bond acceptors, molecular complexity, and fraction sp³ for molecules appearing in JMC 1959-2009.

S4 – Mean and median calculated property values for compounds appearing in JMC 1959-2009



Box plots of molecular weight, calculated logP, topological polar surface area, and rotatable bonds for molecules appearing in JMC 1959-2009.



Box plots of number of hydrogen bond donors, number of hydrogen bond acceptors, molecular complexity, and fraction sp^3 for molecules appearing in JMC 1959-2009.

YEARS	MW	XLOGP	TPSA	ROT	HBD	HBA	COMPLEXITY	FSP3
1959-1964	302.68	2.60	57.50	4.86	1.25	2.67	38.51	0.43
1965-1969	302.67	2.45	62.96	4.88	1.30	2.92	39.56	0.38
1970-1974	316.87	2.67	64.83	4.97	1.30	3.10	40.77	0.39
1975-1979	326.71	2.61	70.52	5.19	1.45	3.41	40.83	0.37
1980-1984	334.92	2.37	75.58	5.30	1.62	3.59	43.33	0.38
1985-1989	351.14	2.24	80.10	5.80	1.65	3.82	44.60	0.39
1990-1994	388.67	2.66	86.30	6.60	1.73	4.11	47.44	0.39
1995-1999	399.20	2.97	85.68	6.65	1.76	4.09	46.65	0.38
2000-2004	403.43	2.83	89.29	6.51	1.83	4.27	47.28	0.36
2005-2009	403.29	3.10	87.05	6.33	1.77	4.24	47.59	0.34

Mean values for molecules appearing in JMC 1959-2009

YEARS	MW	XLOGP	TPSA	ROT	HBD	HBA	COMPLEXITY	FSP3
1959-1964	289.37	2.59	49.85	4	1	2	38	0.41
1965-1969	290.34	2.45	54.86	4	1	3	39	0.35
1970-1974	298.40	2.61	55.12	4	1	3	41	0.36
1975-1979	310.30	2.51	61.19	4	1	3	40	0.35
1980-1984	319.44	2.41	66.37	4	1	3	43	0.37
1985-1989	328.41	2.34	69.20	5	1	3	44	0.36
1990-1994	363.41	2.81	74.32	5	1	4	48	0.38
1995-1999	375.32	3.14	74.60	6	1	4	47	0.36
2000-2004	383.24	3.05	77.84	5	1	4	47	0.33
2005-2009	385.46	3.34	76.82	5	1	4	48	0.32

Median values for molecules appearing in JMC 1959-2009