

Article

# Exploring the Potential of Oleanolic Acid Dimers—Cytostatic and Antioxidant Activities, Molecular Docking, and ADMETox Profile

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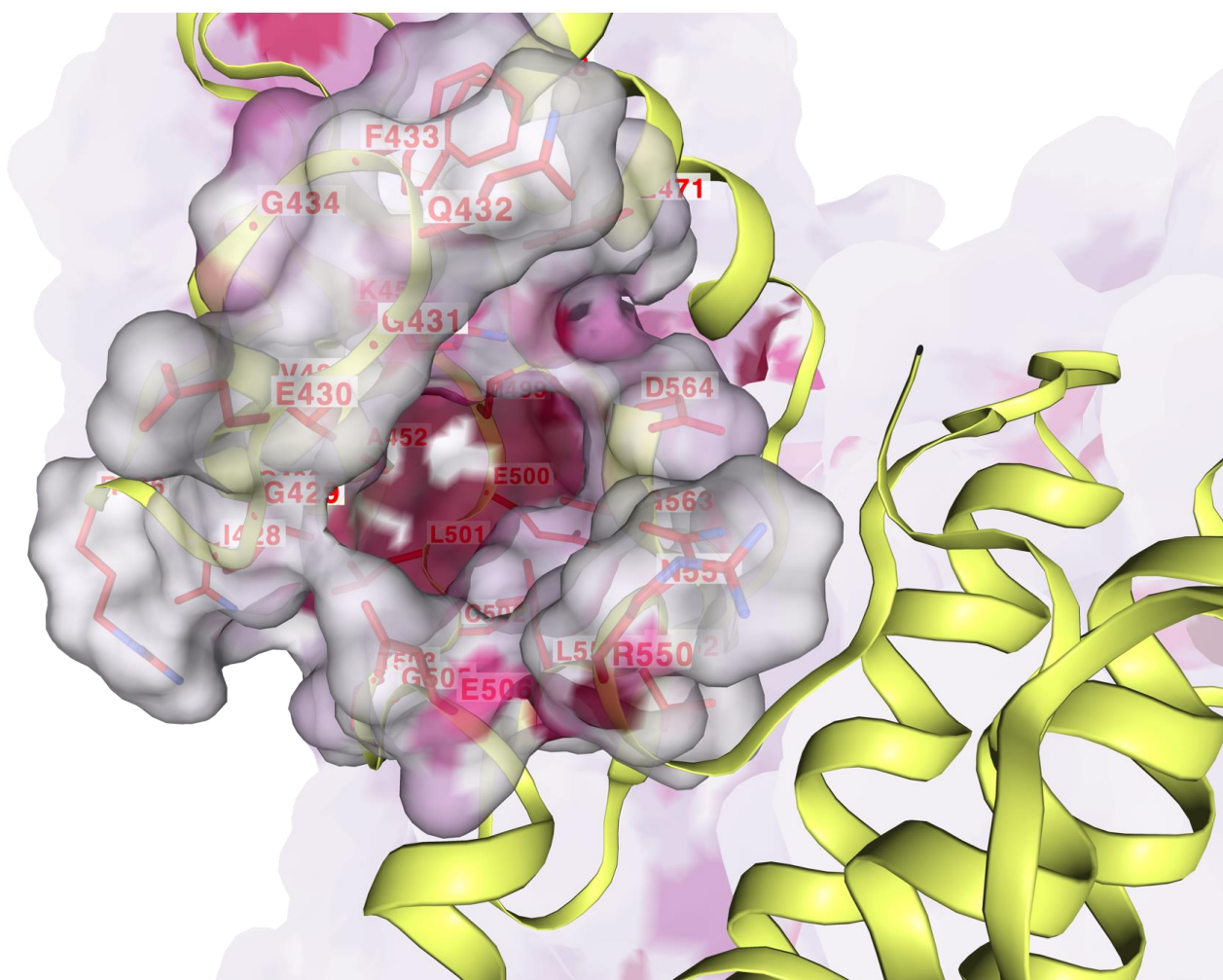
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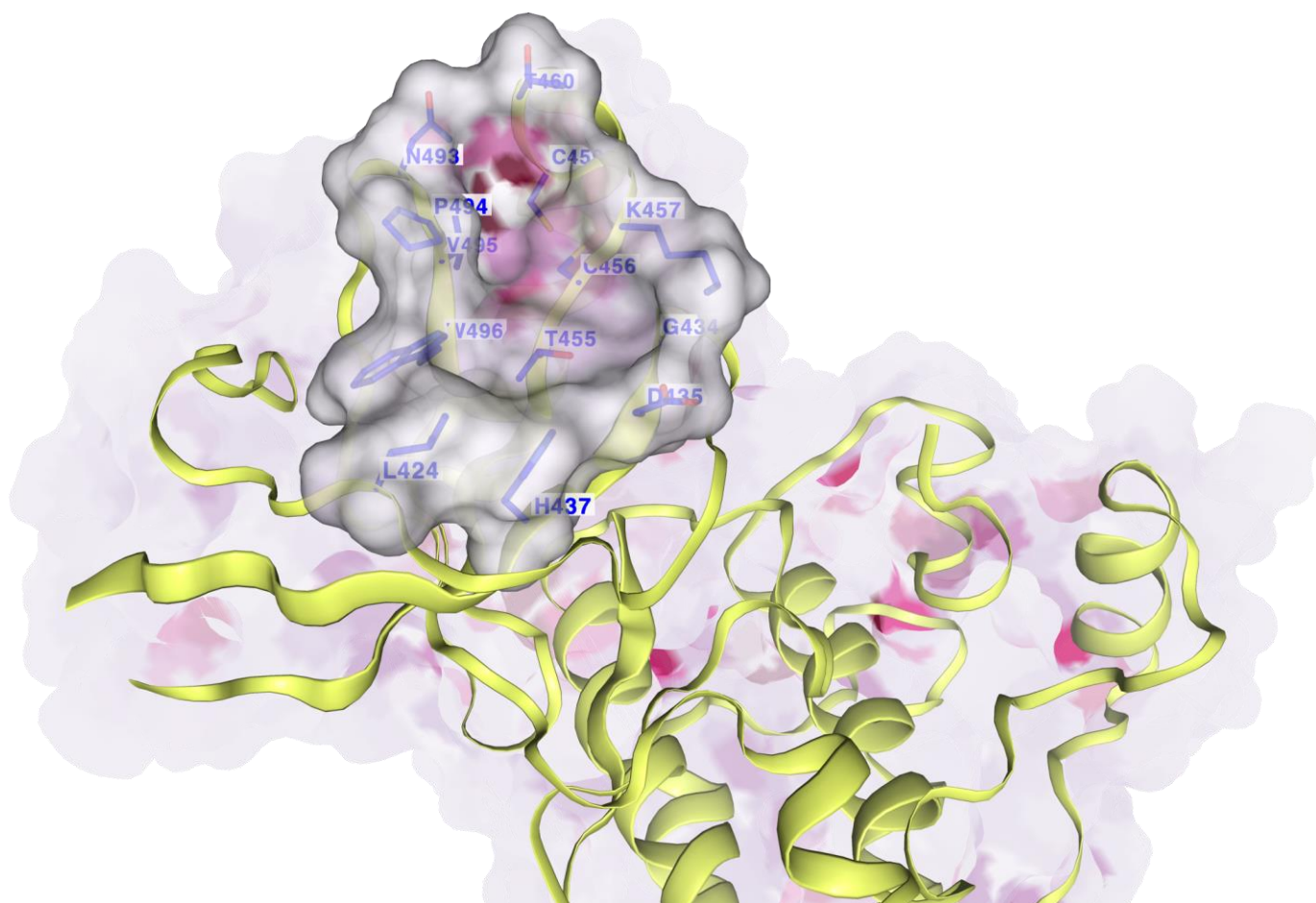
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## Supplementary Materials 01. Cavities of 1MP8

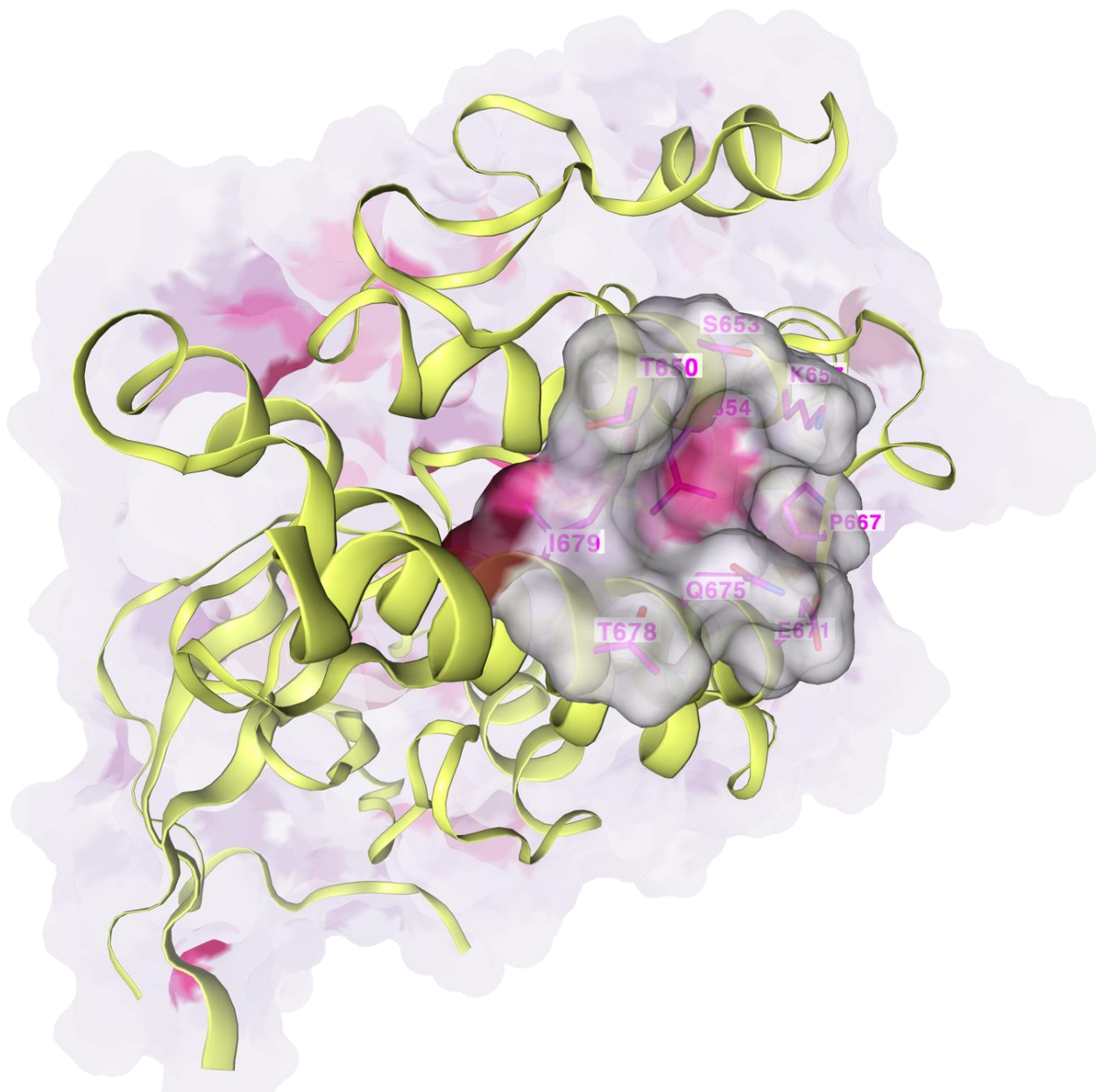
**Figure S1.** Largest Cavity C1 of FAK (PBD ID: 1MP8), with calculated volume 818 Å<sup>3</sup>.



**Figure S2.** Cavity C2 of FAK (PDB ID: 1MP8), with calculated volume 161 Å<sup>3</sup>.

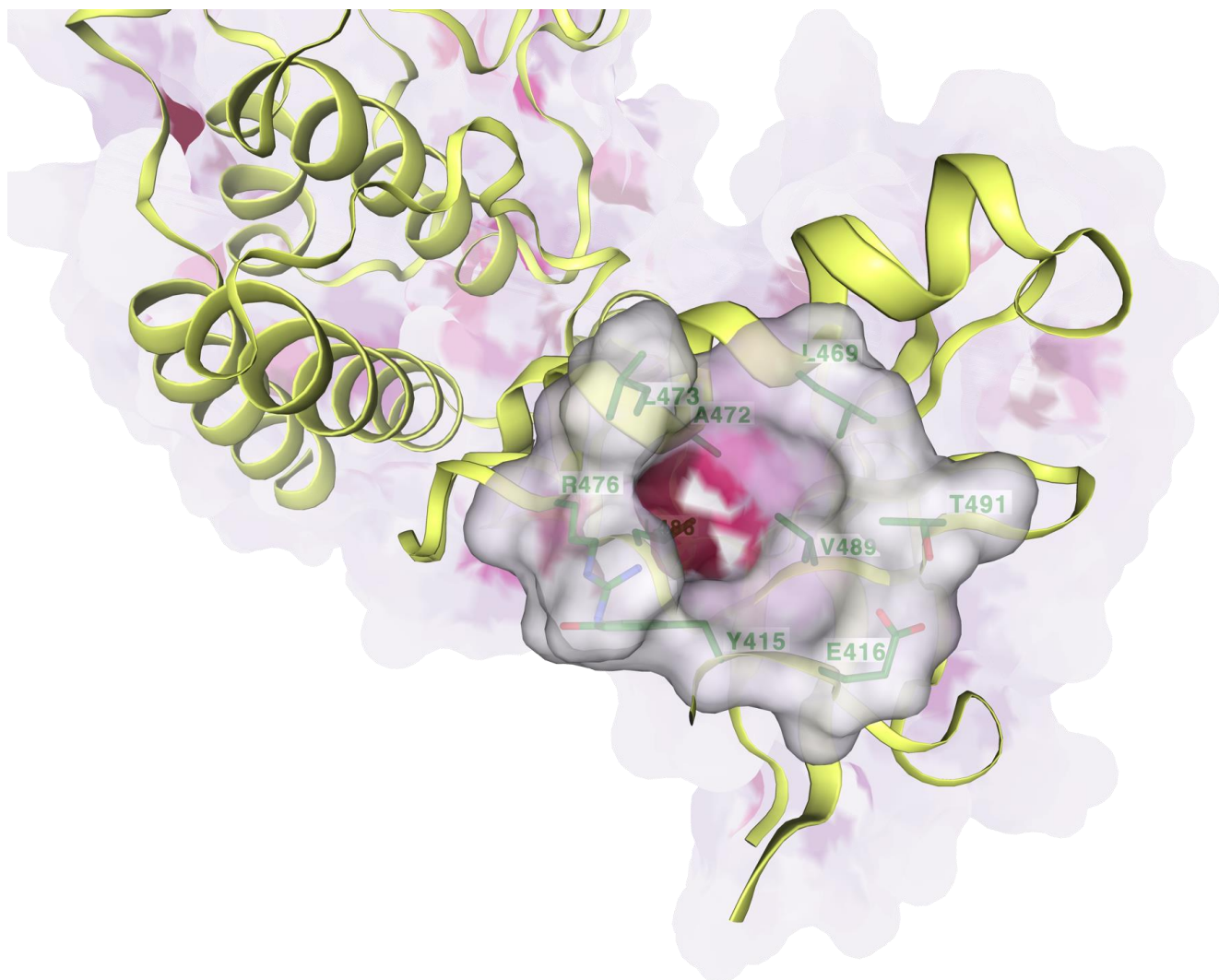


**Figure S3.** Cavity C3 of FAK (PDB ID: 1MP8), with calculated volume 96 Å<sup>3</sup>.

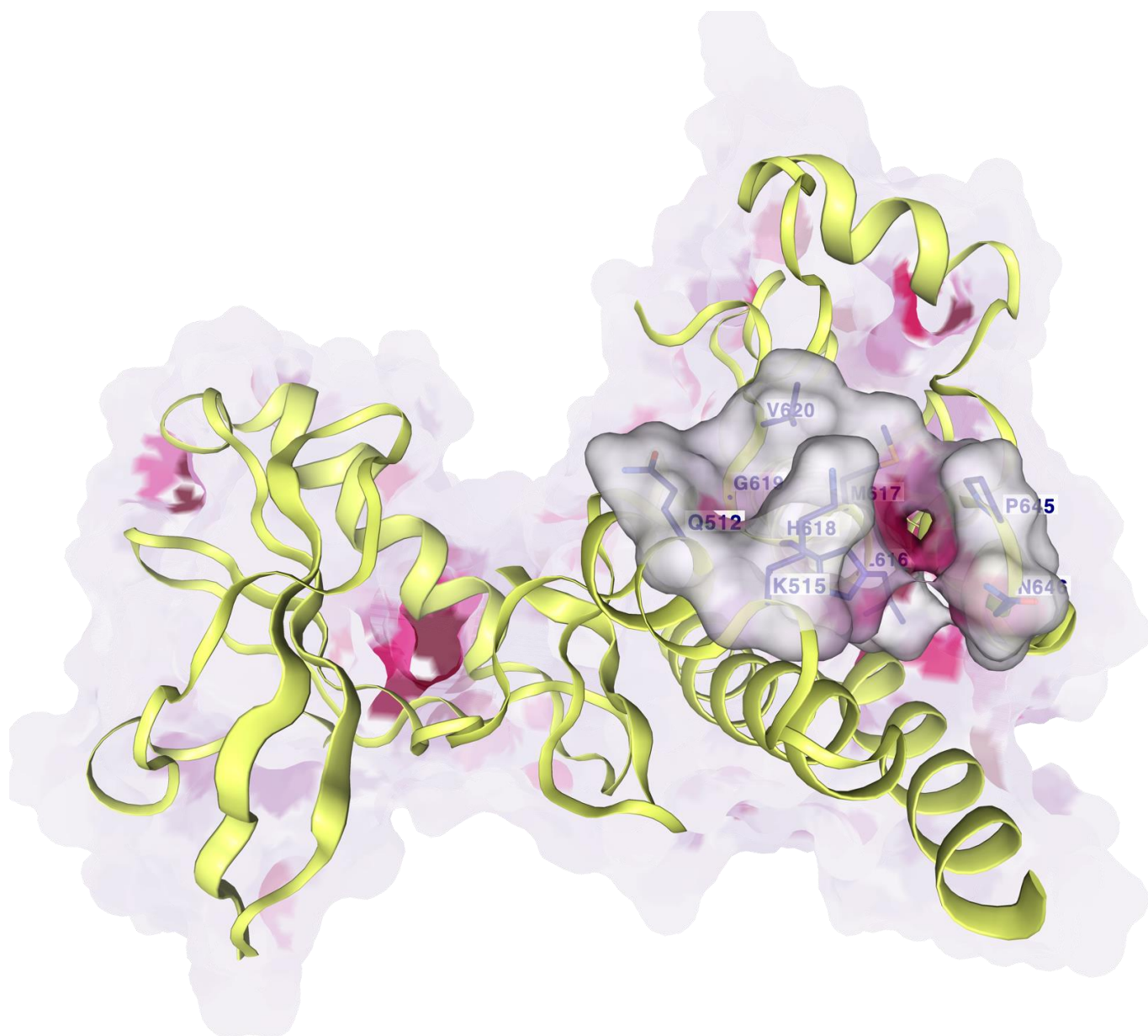




**Figure S4.** Cavity C4 of FAK (PBD ID: 1MP8), with calculated volume 95 Å<sup>3</sup>.



**Figure S5.** Cavity C5 of FAK (PBD ID: 1MP8), with calculated volume 84 Å<sup>3</sup>.



**Table S1.** Vina score in kcal · mol<sup>-1</sup>

	C1	C2	C3	C4	C5
Dimer No.	CurPocket ID	Vina score	Cavity volume (Å <sup>3</sup> )	Center (x, y, z)	Docking size (x, y, z)
2a	C1	-10.8	818	38, -3, 25	30, 30, 30
	C2	-8.6	96	38, 13, -3	30, 30, 30
	C3	-8.5	161	35, -14, 34	30, 30, 30
	C4	-7.9	95	41, -19, 20	30, 30, 30
	C5	-5.8	84	32, 18, 19	30, 30, 30
2b	C1	-9.8	818	38, -3, 25	29, 29, 29
	C2	-7.0	161	35, -14, 34	29, 29, 29
	C3	-7.1	96	38, 13, -3	29, 29, 29
	C4	-7.8	95	41, -19, 20	29, 29, 29
	C5	-6.6	84	32, 18, 19	29, 29, 29
2c	C1	-10.2	818	38, -3, 25	34, 34, 34
	C2	-7.9	161	35, -14, 34	34, 34, 34
	C3	-7.4	96	38, 13, -3	34, 34, 34
	C4	-8.5	95	41, -19, 20	34, 34, 34
	C5	-6.7	84	32, 18, 19	34, 34, 34
2d	C1	-9.6	818	38, -3, 25	30, 30, 30
	C2	-7.0	161	35, -14, 34	30, 30, 30
	C3	-8.2	96	38, 13, -3	30, 30, 30
	C4	-7.9	95	41, -19, 20	30, 30, 30
	C5	-7.4	84	32, 18, 19	30, 30, 30
2e	C1	-9.4	818	38, -3, 25	30, 30, 30
	C2	-8.6	161	35, -14, 34	30, 30, 30
	C3	-7.9	96	38, 13, -3	30, 30, 30
	C4	-8.7	95	41, -19, 20	30, 30, 30
	C5	-8.5	84	32, 18, 19	30, 30, 30
2f	C1	-11.6	818	38, -3, 25	30, 30, 30
	C2	-8.5	95	41, -19, 20	30, 30, 30
	C3	-7.5	161	35, -14, 34	30, 30, 30
	C4	-6.6	96	38, 13, -3	30, 30, 30
	C5	-5.7	84	32, 18, 19	30, 30, 30
2g	C1	-10.6	818	38, -3, 25	35, 35, 35
	C2	-7.4	161	35, -14, 34	35, 35, 35
	C3	-7.2	95	41, -19, 20	35, 35, 35
	C4	-6.5	96	38, 13, -3	35, 35, 35
	C5	-5.9	84	32, 18, 19	35, 35, 35
2h	C1	-9.6	818	38, -3, 25	36, 36, 36
	C2	-7.2	161	35, -14, 34	36, 36, 36
	C3	-7.5	96	38, 13, -3	36, 36, 36
	C4	-8.6	95	41, -19, 20	36, 36, 36
	C5	-7.9	84	32, 18, 19	36, 36, 36
2i	C1	-7.6	818	38, -3, 25	37, 37, 37
	C2	-8.0	161	35, -14, 34	37, 37, 37
	C3	-6.2	96	38, 13, -3	37, 37, 37

2j	C4	-7.9	95	41, -19, 20	37, 37, 37
	C5	-6.8	84	32, 18, 19	37, 37, 37
	C1	-10.4	818	38, -3, 25	36, 36, 36
	C2	-7.4	161	35, -14, 34	36, 36, 36
	C3	-7.0	96	38, 13, -3	36, 36, 36
2k	C4	-7.7	95	41, -19, 20	36, 36, 36
	C5	-6.9	84	32, 18, 19	36, 36, 36
	C1	-8.4	818	38, -3, 25	39, 39, 39
	C2	-6.1	161	35, -14, 34	39, 39, 39
	C3	-6.8	96	38, 13, -3	39, 39, 39
2l	C4	-7.0	95	41, -19, 20	39, 39, 39
	C5	-7.4	84	32, 18, 19	39, 39, 39
	C1	-9.4	818	38, -3, 25	39, 39, 39
	C2	-6.6	161	35, -14, 34	39, 39, 39
	C3	-5.7	96	38, 13, -3	39, 39, 39
2m	C4	-7.8	95	41, -19, 20	39, 39, 39
	C5	-6.1	84	32, 18, 19	39, 39, 39
	C1	-6.4	818	38, -3, 25	43, 43, 43
	C2	-8.2	161	35, -14, 34	43, 43, 43
	C3	-5.1	96	38, 13, -3	43, 43, 43
2n	C4	-7.3	95	41, -19, 20	43, 43, 43
	C5	-5.4	84	32, 18, 19	43, 43, 43
	C1	-8.6	818	38, -3, 25	44, 44, 44
	C2	-6.8	161	35, -14, 34	44, 44, 44
	C3	-5.8	96	38, 13, -3	44, 44, 44
	C4	-8.2	95	41, -19, 20	44, 44, 44
	C5	-6.3	84	32, 18, 19	44, 44, 44