

Supplementary file 2

Calculated masses of potential intermediates in the biosynthesis of cucurbitacins. The first intermediate listed is cucurbitadienol (Formula: C₃₀H₅₀O), precursor for all the Cucs. The rest of the potential intermediates is derived from cucurbitadienol with the addition of 1-9 hydroxyl groups, 1-3 carbonyl groups, an acetyl group and/or the creation of a double bond (listed to the left). To the right in the table the masses (as *m/z*-values) of the potential intermediates is listed, with the loss of a hydrogen atom ([M-H]⁻) and a water molecule ([M-H₂O-H]⁻) and with the addition of a formate adduct ([M+HCOO]⁻). Masses used for calculation: C, 12; H, 1,007825; O, 15,99492; hydroxyl group, 15,99492; carbonyl group, 13,97927; double bond, -2,01565; acetyl group, 42,01057; H₂O, 18,01057; formate adduct, 45.

Hydroxyl	Carbonyl	Double bond	Acetyl	Formula	[M-H] ⁻	[M-H ₂ O-H] ⁻	[M+HCOO] ⁻
0	0	0	0	C30H50O1	425,3784	407,3678	471,3862
1	0	0	0	C30H50O2	441,3733	423,3627	487,3811
2	0	0	0	C30H50O3	457,3682	439,3576	503,3760
3	0	0	0	C30H50O4	473,3631	455,3526	519,3710
4	0	0	0	C30H50O5	489,3581	471,3475	535,3659
5	0	0	0	C30H50O6	505,3530	487,3424	551,3608
6	0	0	0	C30H50O7	521,3479	503,3373	567,3557
7	0	0	0	C30H50O8	537,3428	519,3322	583,3506
8	0	0	0	C30H50O9	553,3377	535,3272	599,3456
9	0	0	0	C30H50O10	569,3327	551,3221	615,3405
0	1	0	0	C30H48O2	439,3576	421,3471	485,3655
1	1	0	0	C30H48O3	455,3526	437,3420	501,3604
2	1	0	0	C30H48O4	471,3475	453,3369	517,3553
3	1	0	0	C30H48O5	487,3424	469,3318	533,3502
4	1	0	0	C30H48O6	503,3373	485,3268	549,3452
5	1	0	0	C30H48O7	519,3322	501,3217	565,3401
6	1	0	0	C30H48O8	535,3272	517,3166	581,3350
7	1	0	0	C30H48O9	551,3221	533,3115	597,3299
8	1	0	0	C30H48O10	567,3170	549,3064	613,3248
0	2	0	0	C30H46O3	453,3369	435,3263	499,3447
1	2	0	0	C30H46O4	469,3318	451,3213	515,3397
2	2	0	0	C30H46O5	485,3268	467,3162	531,3346
3	2	0	0	C30H46O6	501,3217	483,3111	547,3295
4	2	0	0	C30H46O7	517,3166	499,3060	563,3244
5	2	0	0	C30H46O8	533,3115	515,3009	579,3193
6	2	0	0	C30H46O9	549,3064	531,2959	595,3143
7	2	0	0	C30H46O10	565,3014	547,2908	611,3092
0	3	0	0	C30H44O4	467,3162	449,3056	513,3240
1	3	0	0	C30H44O5	483,3111	465,3005	529,3189
2	3	0	0	C30H44O6	499,3060	481,2955	545,3139
3	3	0	0	C30H44O7	515,3009	497,2904	561,3088
4	3	0	0	C30H44O8	531,2959	513,2853	577,3037
5	3	0	0	C30H44O9	547,2908	529,2802	593,2986
6	3	0	0	C30H44O10	563,2857	545,2751	609,2935
0	0	1	0	C30H48O1	423,3627	405,3522	469,3706
1	0	1	0	C30H48O2	439,3576	421,3471	485,3655
2	0	1	0	C30H48O3	455,3526	437,3420	501,3604
3	0	1	0	C30H48O4	471,3475	453,3369	517,3553
4	0	1	0	C30H48O5	487,3424	469,3318	533,3502
5	0	1	0	C30H48O6	503,3373	485,3268	549,3452
6	0	1	0	C30H48O7	519,3322	501,3217	565,3401
7	0	1	0	C30H48O8	535,3272	517,3166	581,3350
8	0	1	0	C30H48O9	551,3221	533,3115	597,3299
9	0	1	0	C30H48O10	567,3170	549,3064	613,3248
0	1	1	0	C30H46O2	437,3420	419,3314	483,3498
1	1	1	0	C30H46O3	453,3369	435,3263	499,3447
2	1	1	0	C30H46O4	469,3318	451,3213	515,3397
3	1	1	0	C30H46O5	485,3268	467,3162	531,3346

4	1	1	0	C30H46O6	501,3217	483,3111	547,3295
5	1	1	0	C30H46O7	517,3166	499,3060	563,3244
6	1	1	0	C30H46O8	533,3115	515,3009	579,3193
7	1	1	0	C30H46O9	549,3064	531,2959	595,3143
8	1	1	0	C30H46O10	565,3014	547,2908	611,3092
0	2	1	0	C30H44O3	451,3213	433,3107	497,3291
1	2	1	0	C30H44O4	467,3162	449,3056	513,3240
2	2	1	0	C30H44O5	483,3111	465,3005	529,3189
3	2	1	0	C30H44O6	499,3060	481,2955	545,3139
4	2	1	0	C30H44O7	515,3009	497,2904	561,3088
5	2	1	0	C30H44O8	531,2959	513,2853	577,3037
6	2	1	0	C30H44O9	547,2908	529,2802	593,2986
7	2	1	0	C30H44O10	563,2857	545,2751	609,2935
0	3	1	0	C30H42O4	465,3005	447,2900	511,3084
1	3	1	0	C30H42O5	481,2955	463,2849	527,3033
2	3	1	0	C30H42O6	497,2904	479,2798	543,2982
3	3	1	0	C30H42O7	513,2853	495,2747	559,2931
4	3	1	0	C30H42O8	529,2802	511,2696	575,2880
5	3	1	0	C30H42O9	545,2751	527,2646	591,2830
6	3	1	0	C30H42O10	561,2701	543,2595	607,2779
0	0	0	1	C32H52O2	467,3889	449,3784	513,3968
1	0	0	1	C32H52O3	483,3839	465,3733	529,3917
2	0	0	1	C32H52O4	499,3788	481,3682	545,3866
3	0	0	1	C32H52O5	515,3737	497,3631	561,3815
4	0	0	1	C32H52O6	531,3686	513,3581	577,3765
5	0	0	1	C32H52O7	547,3635	529,3530	593,3714
6	0	0	1	C32H52O8	563,3585	545,3479	609,3663
7	0	0	1	C32H52O9	579,3534	561,3428	625,3612
8	0	0	1	C32H52O10	595,3483	577,3377	641,3561
9	0	0	1	C32H52O11	611,3432	593,3327	657,3511
0	1	0	1	C32H50O3	481,3682	463,3576	527,3760
1	1	0	1	C32H50O4	497,3631	479,3526	543,3710
2	1	0	1	C32H50O5	513,3581	495,3475	559,3659
3	1	0	1	C32H50O6	529,3530	511,3424	575,3608
4	1	0	1	C32H50O7	545,3479	527,3373	591,3557
5	1	0	1	C32H50O8	561,3428	543,3322	607,3506
6	1	0	1	C32H50O9	577,3377	559,3272	623,3456
7	1	0	1	C32H50O10	593,3327	575,3221	639,3405
8	1	0	1	C32H50O11	609,3276	591,3170	655,3354
0	2	0	1	C32H48O4	495,3475	477,3369	541,3553
1	2	0	1	C32H48O5	511,3424	493,3318	557,3502
2	2	0	1	C32H48O6	527,3373	509,3268	573,3452
3	2	0	1	C32H48O7	543,3322	525,3217	589,3401
4	2	0	1	C32H48O8	559,3272	541,3166	605,3350
5	2	0	1	C32H48O9	575,3221	557,3115	621,3299
6	2	0	1	C32H48O10	591,3170	573,3064	637,3248
7	2	0	1	C32H48O11	607,3119	589,3014	653,3198
0	3	0	1	C32H46O5	509,3268	491,3162	555,3346
1	3	0	1	C32H46O6	525,3217	507,3111	571,3295
2	3	0	1	C32H46O7	541,3166	523,3060	587,3244
3	3	0	1	C32H46O8	557,3115	539,3009	603,3193
4	3	0	1	C32H46O9	573,3064	555,2959	619,3143
5	3	0	1	C32H46O10	589,3014	571,2908	635,3092
6	3	0	1	C32H46O11	605,2963	587,2857	651,3041
0	0	1	1	C32H50O2	465,3733	447,3627	511,3811
1	0	1	1	C32H50O3	481,3682	463,3576	527,3760
2	0	1	1	C32H50O4	497,3631	479,3526	543,3710
3	0	1	1	C32H50O5	513,3581	495,3475	559,3659
4	0	1	1	C32H50O6	529,3530	511,3424	575,3608

5	0	1	1	C32H5007		545,3479	527,3373	591,3557
6	0	1	1	C32H5008		561,3428	543,3322	607,3506
7	0	1	1	C32H5009		577,3377	559,3272	623,3456
8	0	1	1	C32H50010		593,3327	575,3221	639,3405
9	0	1	1	C32H50011		609,3276	591,3170	655,3354
0	1	1	1	C32H4803		479,3526	461,3420	525,3604
1	1	1	1	C32H4804		495,3475	477,3369	541,3553
2	1	1	1	C32H4805		511,3424	493,3318	557,3502
3	1	1	1	C32H4806		527,3373	509,3268	573,3452
4	1	1	1	C32H4807		543,3322	525,3217	589,3401
5	1	1	1	C32H4808		559,3272	541,3166	605,3350
6	1	1	1	C32H4809		575,3221	557,3115	621,3299
7	1	1	1	C32H48010		591,3170	573,3064	637,3248
8	1	1	1	C32H48011		607,3119	589,3014	653,3198
0	2	1	1	C32H4604		493,3318	475,3213	539,3397
1	2	1	1	C32H4605		509,3268	491,3162	555,3346
2	2	1	1	C32H4606		525,3217	507,3111	571,3295
3	2	1	1	C32H4607		541,3166	523,3060	587,3244
4	2	1	1	C32H4608		557,3115	539,3009	603,3193
5	2	1	1	C32H4609		573,3064	555,2959	619,3143
6	2	1	1	C32H46010		589,3014	571,2908	635,3092
7	2	1	1	C32H46011		605,2963	587,2857	651,3041
0	3	1	1	C32H4405		507,3111	489,3005	553,3189
1	3	1	1	C32H4406		523,3060	505,2955	569,3139
2	3	1	1	C32H4407		539,3009	521,2904	585,3088
3	3	1	1	C32H4408		555,2959	537,2853	601,3037
4	3	1	1	C32H4409		571,2908	553,2802	617,2986
5	3	1	1	C32H44010		587,2857	569,2751	633,2935
6	3	1	1	C32H44011		603,2806	585,2701	649,2885