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Supporting Information of

Sequential analysis for identification of byproduct from N-benzylation reaction: Wound healing and anti-inflammatory potential in byproduct 4-chlorobenzyl 2-((4-chlorobenzyl)amino) benzoate

Sequential analysis for identification of byproduct from N-benzylation reaction: Wound healing and anti-inflammatory potential in byproduct 4-chlorobenzyl 2-((4-chlorobenzyl)amino) benzoate

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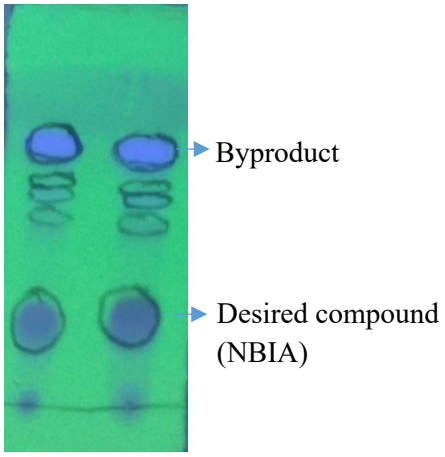

Figure S1. TLC* image of crude compound (NaH, 30°C)

NBIA- N-benzylated isatoic anhydride

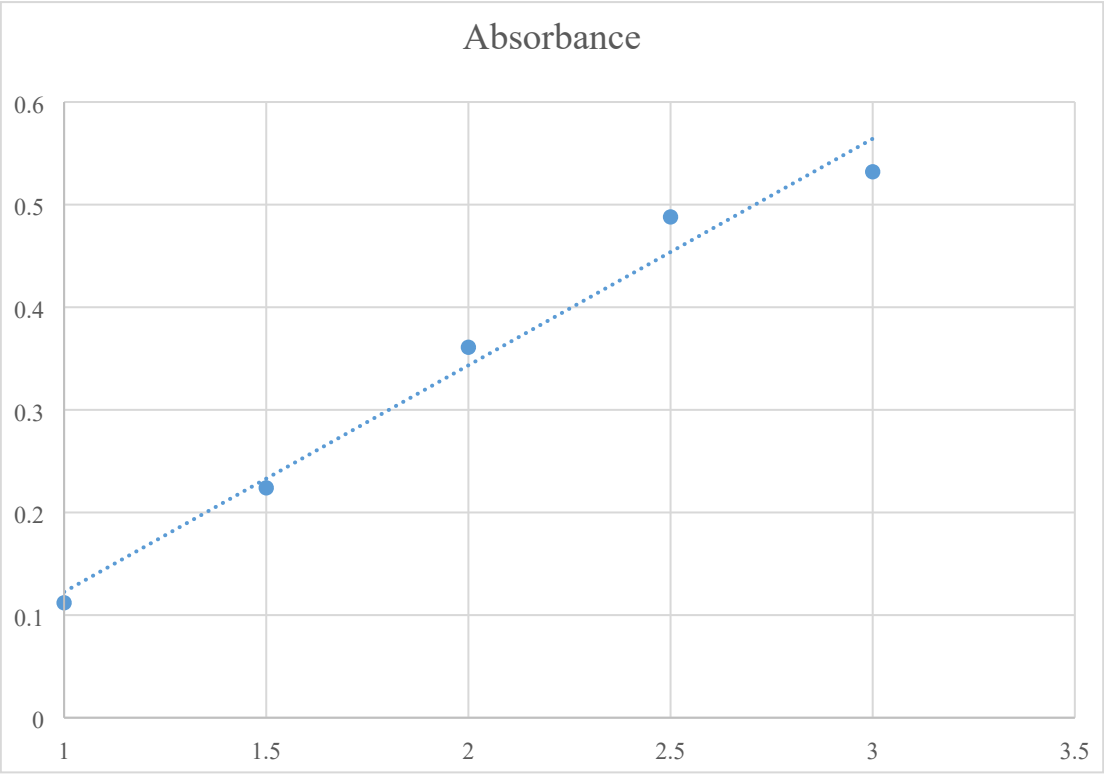

Figure S2. Standard curve for Hydroxyproline

Table S1. Crystal data and structure refinement for CCAB.

Identification code	M
Empirical formula	$C_{21}H_{17}Cl_2NO_2$
Formula weight	386.26
Temperature/K	296.15
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.168(8)
b/Å	5.683(3)
c/Å	21.306(11)
α/°	90
β/°	100.272(9)
γ/°	90
Volume/Å^3	1807.1(16)
Z	4
ρ_{calc}g/cm^3	1.420
μ/mm^{-1}	0.375
F(000)	800.0
Crystal size/mm^3	0.36 × 0.22 × 0.2
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	8.034 to 58.276
Index ranges	$-16 \leq h \leq 20$, $-7 \leq k \leq 7$, $-28 \leq l \leq 23$
Reflections collected	7043
Independent reflections	4330 [R_{int} = 0.0496, R_{sigma} = 0.0887]
Data/restraints/parameters	4330/0/239
Goodness-of-fit on F^2	0.897
Final R indexes [I>=2σ (I)]	R_1 = 0.0598, wR_2 = 0.1454
Final R indexes [all data]	R_1 = 0.1098, wR_2 = 0.1803
Largest diff. peak/hole / e Å^{-3}	0.30/-0.40

Table S2 .Interatomic distances (Å) of 4-chlorobenzyl 2-((4-chlorobenzyl)amino)

benzoate

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cl1	C1	1.754(3)	C8	C9	1.470(4)
Cl2	C19	1.737(3)	C9	C10	1.411(4)
O1	C7	1.439(4)	C9	C14	1.421(4)
O1	C8	1.345(3)	C10	C11	1.377(4)
O2	C8	1.223(3)	C11	C12	1.392(4)
N1	C14	1.373(4)	C12	C13	1.380(4)
N1	C15	1.451(4)	C13	C14	1.404(4)
C1	C2	1.376(4)	C15	C16	1.511(4)
C1	C6	1.380(4)	C16	C17	1.396(4)
C2	C3	1.389(4)	C16	C21	1.393(4)
C3	C4	1.384(4)	C17	C18	1.388(5)
C4	C5	1.389(4)	C18	C19	1.386(4)
C4	C7	1.508(4)	C19	C20	1.373(4)
C5	C6	1.380(4)	C20	C21	1.386(4)

Table S3. Bond Angles (degree) of 4-chlorobenzyl 2-((4-chlorobenzyl)amino)benzoate

Atom	Atom	Atom	Angle/°
C8	O1	C7	116.2(2)
C14	N1	C15	122.7(3)
C2	C1	Cl1	119.3(2)
C2	C1	C6	121.6(3)
C6	C1	Cl1	119.0(2)
C1	C2	C3	118.7(3)
C4	C3	C2	121.0(3)
C3	C4	C5	118.8(3)
C3	C4	C7	123.6(3)
C5	C4	C7	117.6(3)
C6	C5	C4	121.0(3)
C5	C6	C1	118.8(3)
O1	C7	C4	109.1(2)
O1	C8	C9	112.4(2)
O2	C8	O1	121.6(3)
O2	C8	C9	125.9(3)
C10	C9	C8	119.3(3)
C10	C9	C14	119.1(3)
C14	C9	C8	121.6(3)
C11	C10	C9	121.9(3)
C10	C11	C12	118.7(3)
C13	C12	C11	120.9(3)
C12	C13	C14	121.6(3)
N1	C14	C9	121.4(3)
N1	C14	C13	120.8(3)
C13	C14	C9	117.8(3)
N1	C15	C16	115.0(3)
C17	C16	C15	119.5(3)
C21	C16	C15	122.7(3)
C21	C16	C17	117.9(3)
C18	C17	C16	121.1(3)

C19	C18	C17	119.3(3)
C18	C19	Cl2	119.3(2)
C20	C19	Cl2	119.8(3)
C20	C19	C18	120.9(3)
C19	C20	C21	119.4(3)
C20	C21	C16	121.5(3)

Table S4. Wound Contraction (mm) data of negative control, 10%, 5% formulation and standard (0.2%) groups

S. No.	Group	Time (Days)										
		0	**2**	**4**	**6**	**8**	**10**	**12**	**14**	**16**	**18**	**20**
I	**Negative control**	214.83±2.041	178.50±11.467	165.50±9.586	150.83±8.424	137.33±10.708	127.67±7.062	116±4.336	94.67±21.979	75.00±16.432	13.50±1.871	4.00±6.229
II	**10 %**	209.17±9.326^{NS}	174.83±13.394^{NS}	145.67±13.736^{NS}	123.33±8.454**	91.83±18.798**	69.97±14.787**	64.17±15.497**	21.83±9.152**	2.00±1.897**	0±0^{NS}	0±0^{NS}
III	**5%**	211.17±6.795^{NS}	177.67±15.384^{NS}	155.83±15.381^{NS}	112.83±17.759**	73.67±9.522**	59.00±7.925**	40.33±10.727**	24.33±5.317**	12.67±2.160**	0±0^{NS}	0±0^{NS}
IV	**Std 0.2%**	213.33±1.966^{NS}	164.17±12.205^{NS}	144.00±8.764**	110.50±10.56**	85.50±10.858**	45.50±6.745**	15.50±4.370**	2.00±2.530**	0±0^{NS}	0±0^{NS}	0±0^{NS}

Values are expressed as MEAN±SD at n=6, One way ANOVA followed by Bonferroni test, *P<0.050, **P<0.001 and ^{NS}P>0.001 compared to the negative control