

Table S1 ¹H and ¹³C data of NA dissolved in CDCl₃.

| Carbon no. | δ C | δ H | HMBC (H—C) |
|------------|------------|-------------------------|---|
| 1 | 40.13 t | | |
| 2 | 27.97 t | | |
| 3 | 78.57 d | 3.47 dd (10.5, 5.5) | C ₂ , C ₄ , C ₂₃ , C ₂₄ |
| 4 | 40.33 s | | |
| 5 | 55.97 d | 0.78 dd (11.0, 1.5) | |
| 6 | 18.97 t | | |
| 7 | 34.63 t | | |
| 8 | 41.03 s | | |
| 9 | 49.07 d | 1.56 m | C ₅ , C ₈ , C ₁₀ , C ₁₁ |
| 10 | 38.22 s | | |
| 11 | 23.78 t | 1.98 dd (11.0, 3.81) | C ₁₂ , C ₁₃ |
| 12 | 121.75 d | 5.51 t (3.5) | C ₉ , C ₁₁ , C ₁₃ |
| 13 | 145.32 s | | |
| 14 | 43.36 s | | |
| 15 | 27.97 t | | |
| 16 | 25.33 t | | |
| 17 | 33.97 | | |
| 18 | 54.11 d | 2.66 d (11.0) | C ₁₂ , C ₁₃ , C ₁₇ , C ₁₉ , C ₂₉ |
| 19 | 49.07 d | 1.84 dd (11.0, 11.0) | C ₁₈ , C ₂₀ , C ₂₁ , C ₂₉ , C ₃₀ |
| 20 | 40.49 d | | |
| 21 | 32.28 t | | |
| 22 | 38.09 t | 1.96 m | |
| 23 | 27.69 q | 1.24 s | |
| 24 | 17.47 q | 0.97 s | C ₃ , C ₄ , C ₅ |
| 25 | 17.32 q | 0.90 s | C ₅ , C ₉ |
| 26 | 18.08 q | 1.04 s | |
| 27 | 24.52 q | 1.26 s | |
| 28 | 18.01 | 1.07 s | |
| 29 | 180.54 s | | |
| 30 | 22.08 | 1.01 s | |

Note: δ represents chemical shifts in ppm, s=singlet; d=duplet; m=multiplet; Q=quaternary. *J* values (Hz) are given in parentheses.

Table S2 Binding affinities of ligands for target proteins. Amino acid residues are involved in the binding pocket interactions with NA.

| Proteins | Doxoru bicin | Lipatini b | Vincristi ne | NA | Amino acid residues involved in the binding pocket interactions with NA |
|----------|-----------------|---------------|-----------------|------|---|
| BAX | -9.0 | -8.9 | -7.6 | -8.5 | ASP (A:53), THR(A:56), GLN(A:32), GLN(A:28). LYS(A:57), SER(A:60), TYR(B:163), LYS(A:64), GLU(A:61), GLY(A:29) LEU(A:25), PRO(A:51), , GLN(A:28), GLN(A:32) |
| BCL-2 | -8.5 | -7.1 | -7.3 | -8.2 | ARG(A:45), GLY(A:85), TYR(A:140), TYR(A:39),GLY(A:42), CYS(A:141), LEU(A:88), VAL(A:144), TRP(A:84) |
| NF-κB | -2.0 | -2.0 | -1.8 | -1.9 | ASP(B:129), PRO(B:127), LYS(B:128) |
| P53 | -7.6 | -7.7 | -6.4 | -8.4 | THR(A:329), PHE(A:328), LEU(A:330), ASN(A:345), HOH(A:1004), LEU(A:348), LEU(A:344) PHE(A:341), ILE(A:332), PHE(A:338) |

Note: Binding energy (E-value) is represented as kcal/mol.

Table S3. Effect of NA on hematological parameters.

| Groups | RBCs (×10 ⁶)/μl | WBCs (×10 ³) /μl | Platelets (×10 ³) /μl | Hb (g/dl) | ESR (mm/h) |
|---------------------|--------------------------------|---------------------------------|--------------------------------------|-------------------------|-------------------------|
| Control | 5.93±0.48 ^d | 3.93±0.32 ^d | 514.81±4.28 ^e | 12.33±0.79 ^e | 3.97±0.25 ^c |
| Vehicle (10 % DMSO) | 6.08±0.78 ^e | 3.81±0.45 ^d | 499.81±4.58 ^d | 12.45±0.91 ^e | 4.02±0.45 ^c |
| BPA (50 mg/kg) | 3.88±0.25 ^a | 7.37±0.35 ^a | 308.67±2.51 ^a | 6.57±0.12 ^d | 9.19±0.61 ^a |
| NA (10 mg/kg) | 5.89±0.11 ^d | 4.09±0.15 ^c | 494.8±7.58 ^a | 12.03±0.83 ^d | 4.01±0.41 ^c |
| BPA+NA (10 mg/kg) | 5.62±0.19 ^c | 4.19±0.11 ^c | 468.1±9.81 ^c | 11.33±0.47 ^c | 4.18±0.53 ^{bc} |
| BPA+NA (05 mg/kg) | 5.18±0.13 ^b | 4.76±0.12 ^b | 437±03.21 ^b | 10.31±0.54 ^b | 5.09±0.19 ^b |

Note: Results are presented as mean±SD (n=7). Means with different superscript (^{a-e}) letters in the column are significantly ($p < 0.05$) different from one another.

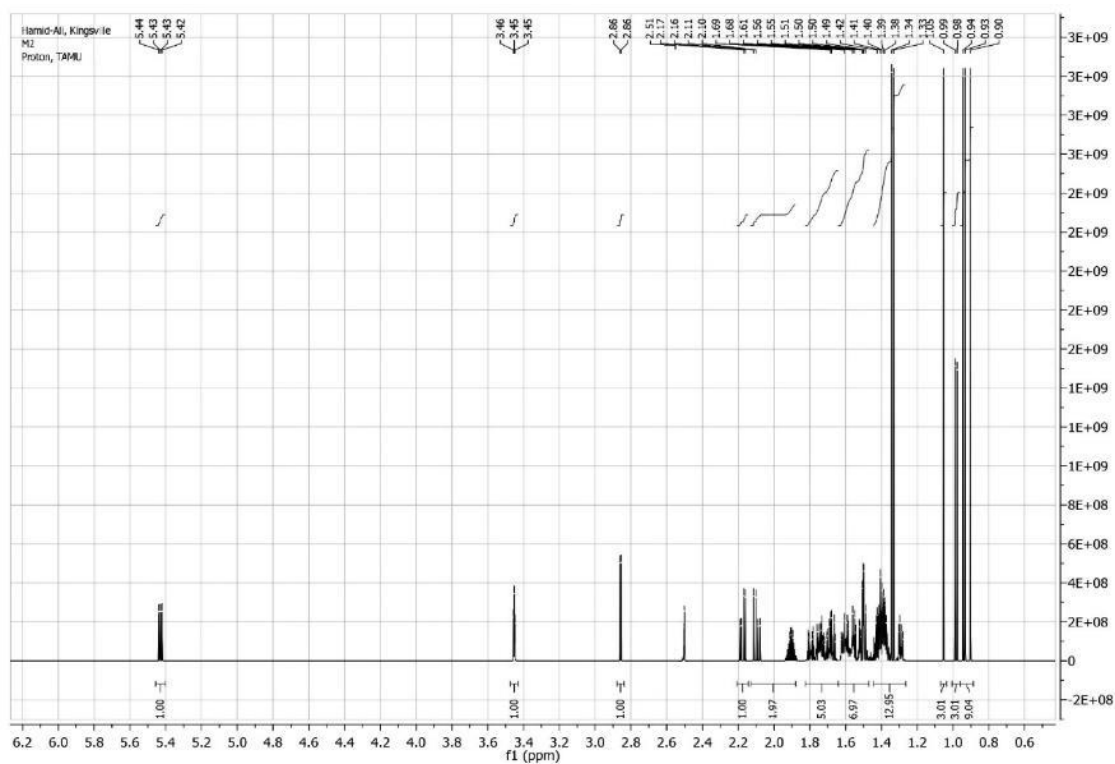


Figure S1 ^1H spectrum (600 MHz, in $\text{DMSO-}d_6$) of NA.

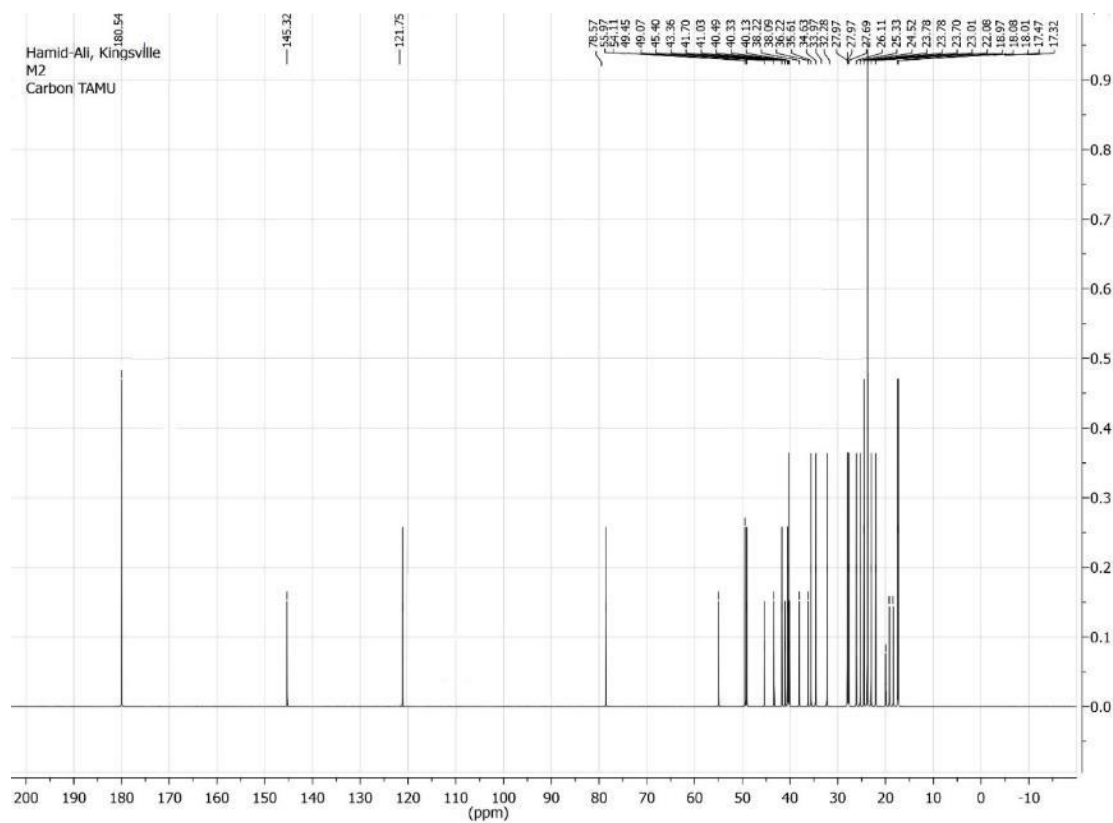


Figure S2 ^{13}C (300 MHz, in $\text{DMSO-}d_6$) spectrum of NA.

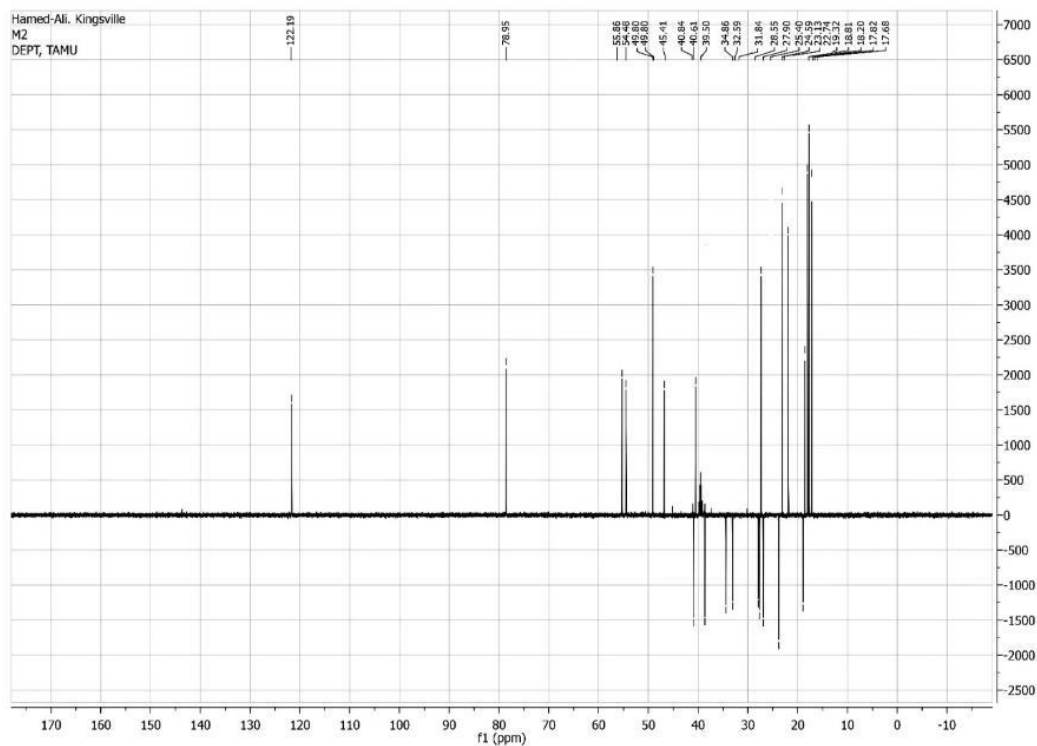


Figure S3 DEPT spectrum (300 MHz, in DMSO- d_6) of NA.

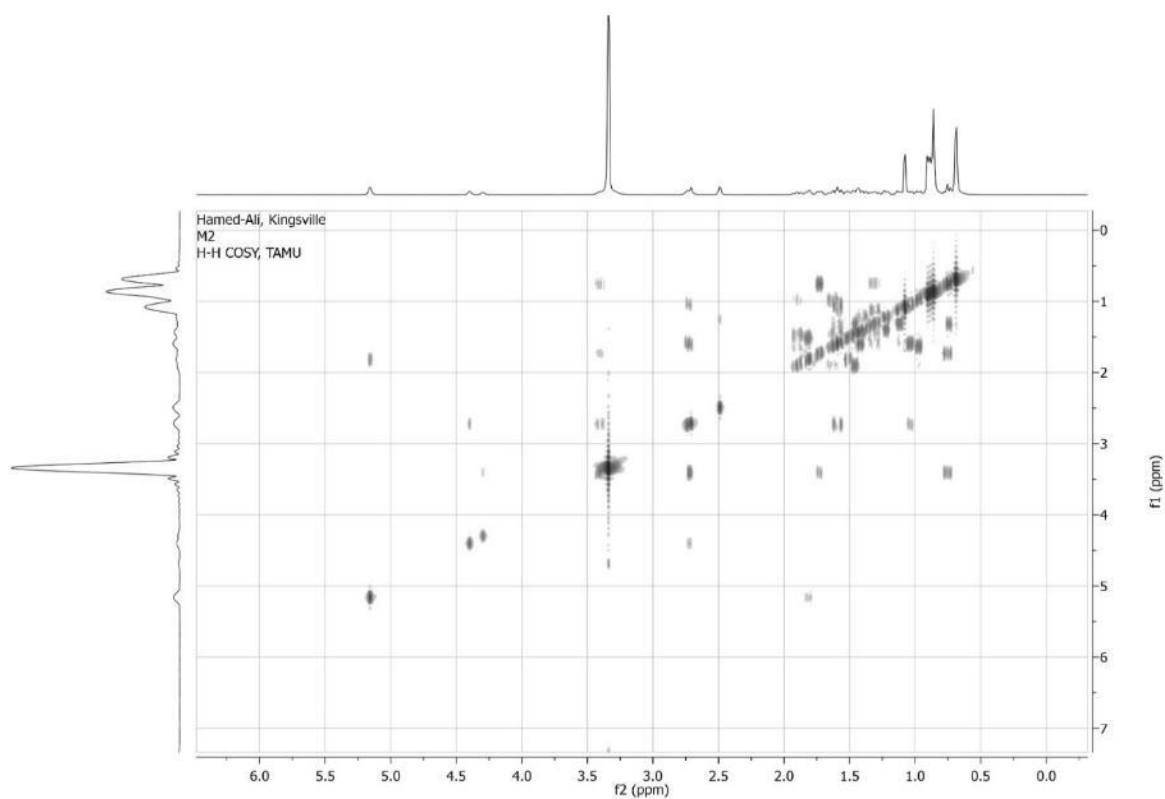


Figure S4 H-H COSY spectrum (600 MHz, in DMSO- d_6) of NA.

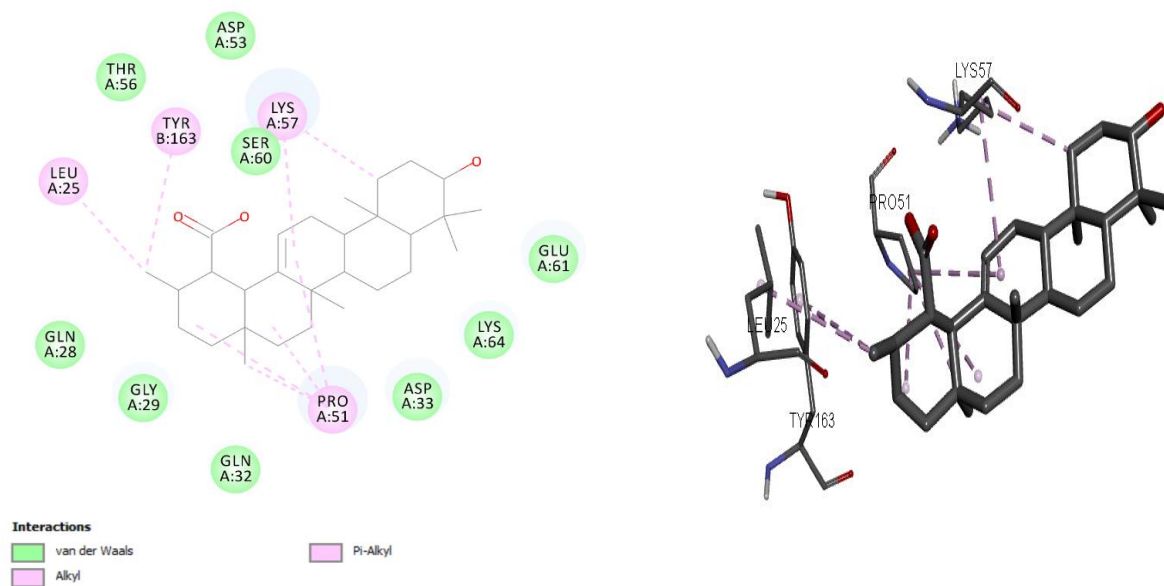


Figure S5 Representation of docked ligand with BAX (PDB-ID: 2K7W)

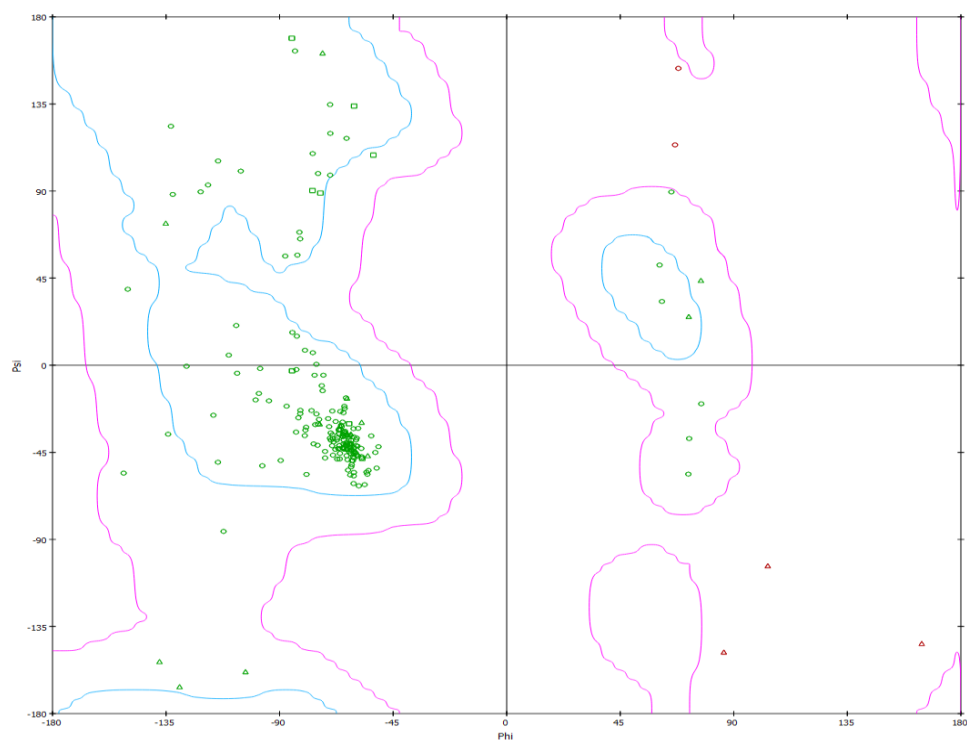


Figure S6 Ramachandran plot confirming that 96 % amino acids are in the allowed regions for the phi (ϕ) and psi (ψ) angles.

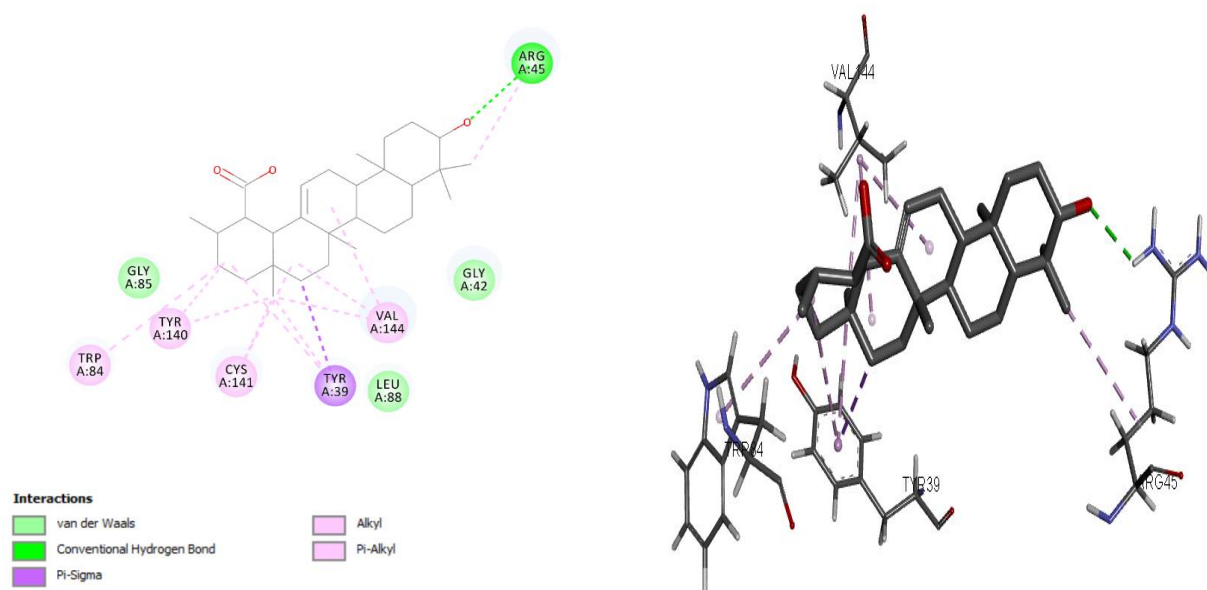


Figure S7 Representation of docked ligand with BCL-2 (PDB-ID 1K3K)

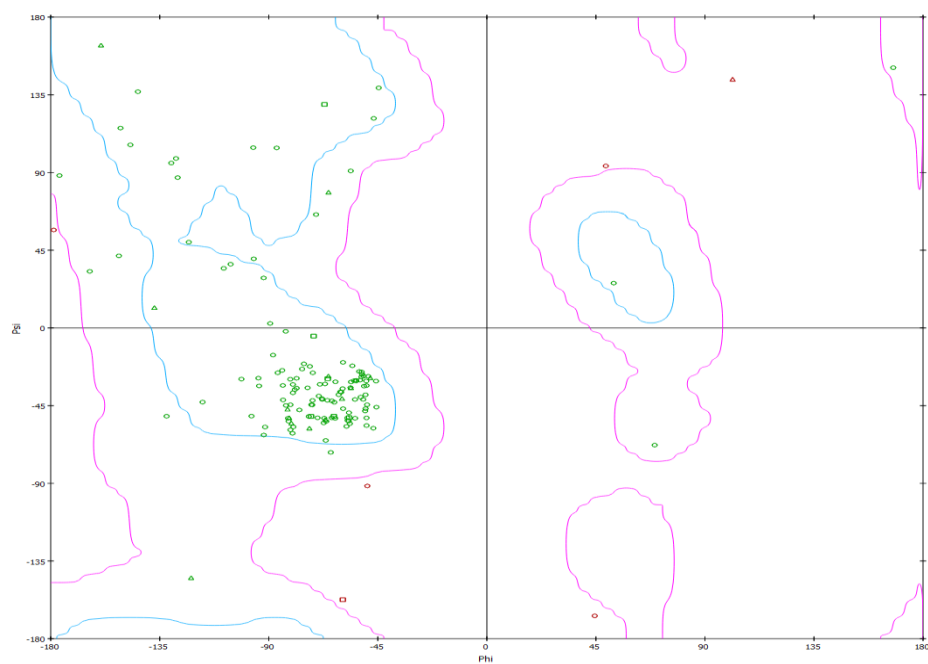


Figure S8 Ramachandran plot confirming that 96 % amino acids are in the allowed regions for the phi (ϕ) and psi (ψ) angles.

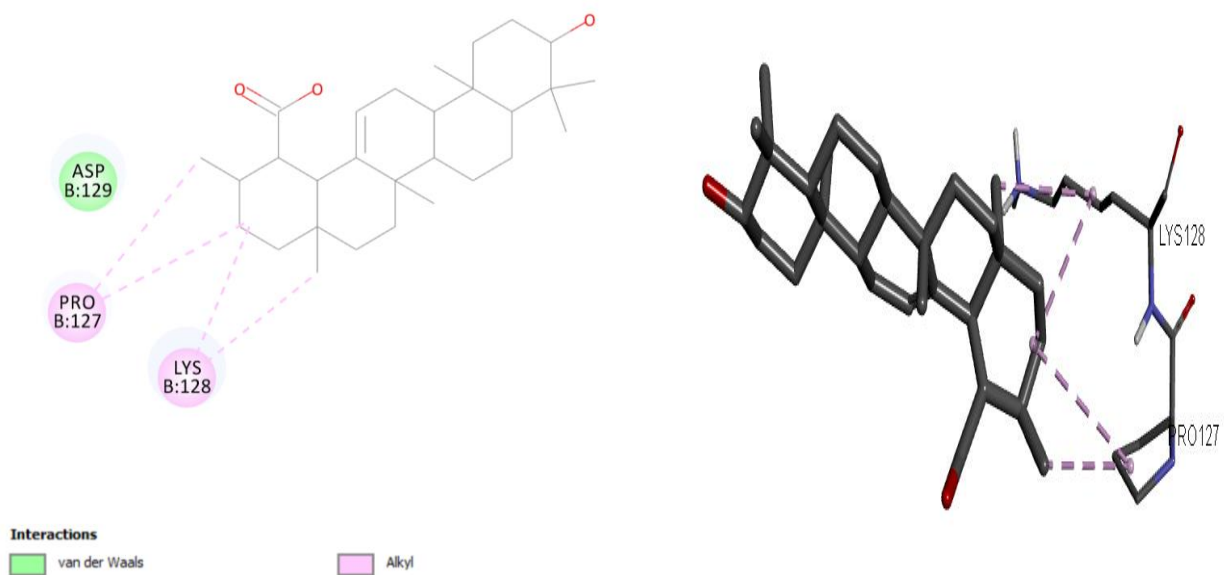


Figure S9 Representation of docked ligand with NF-kB (PDB-ID 1NFK)

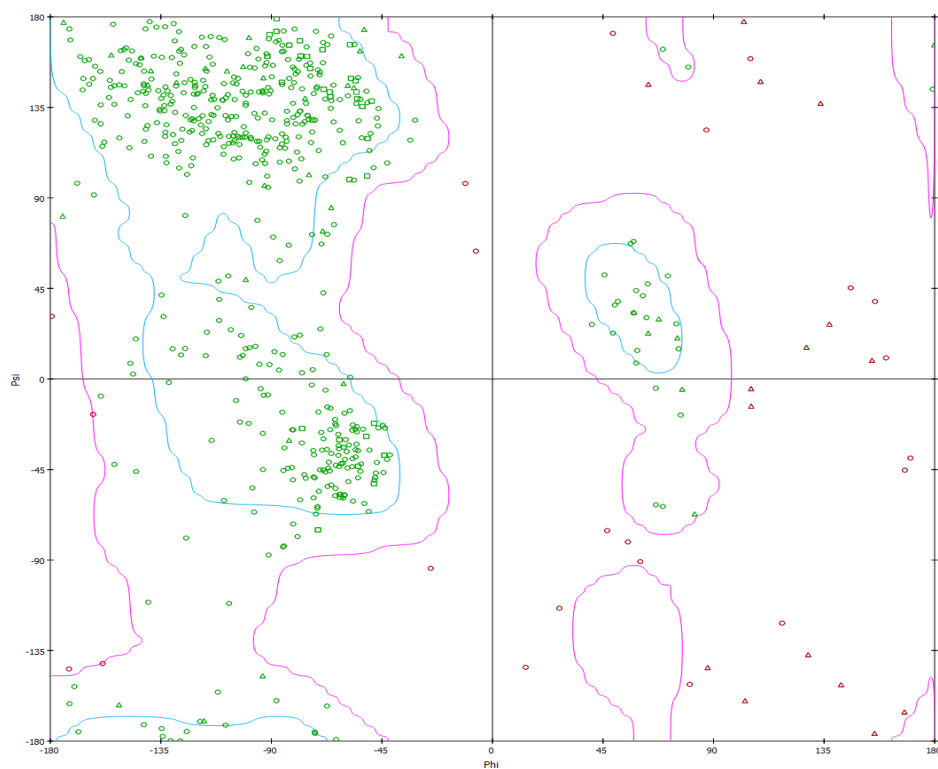


Figure S10 Ramachandran plot confirming that 96 % amino acids are in the allowed regions for the phi (ϕ) and psi (ψ) angles.

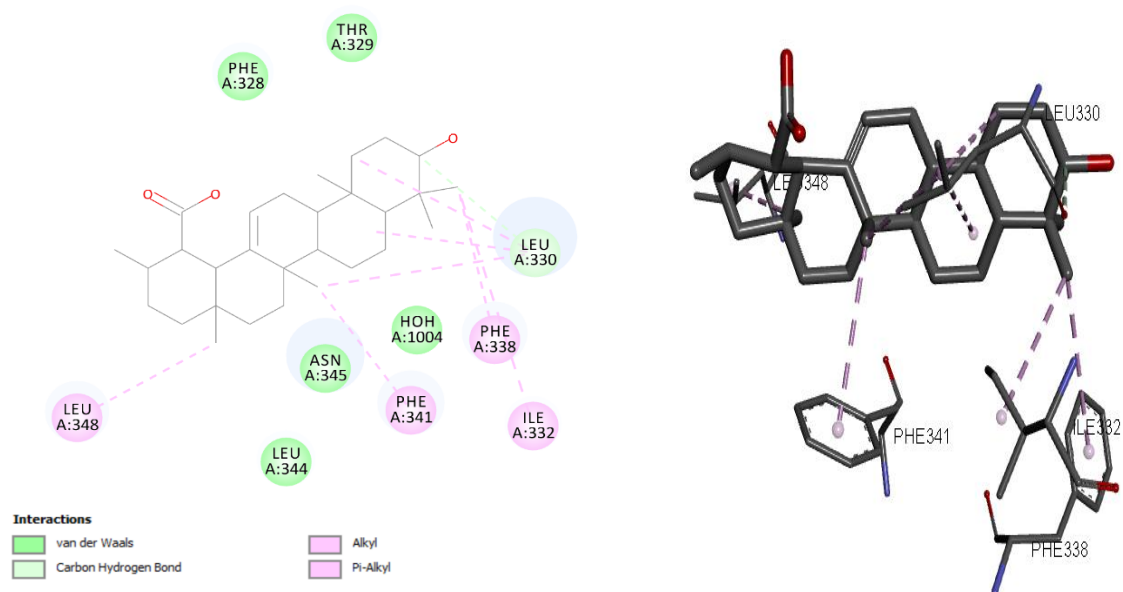


Figure S11 Representation of docked ligand with P53 (PDB-ID 1AIE)

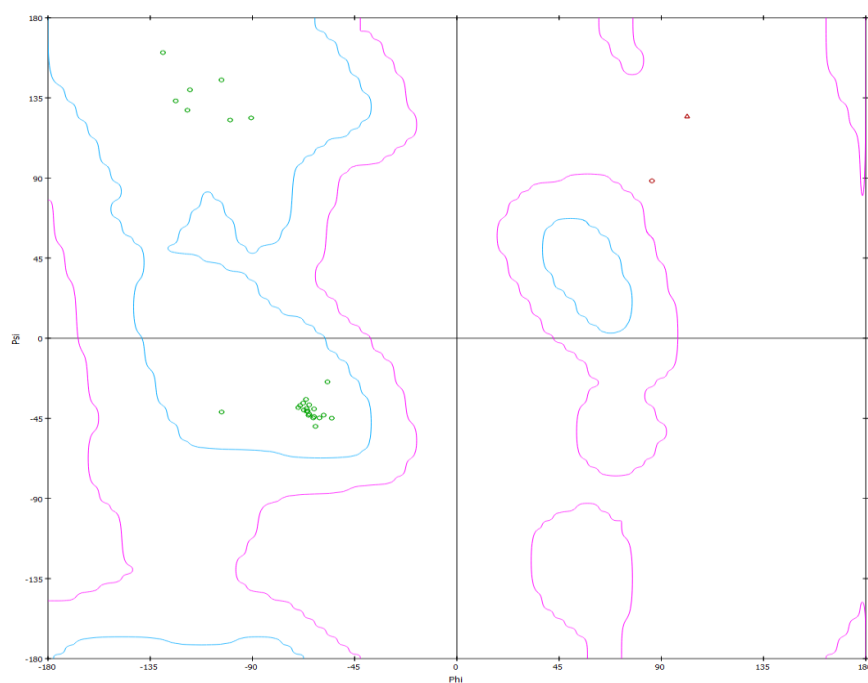


Figure S12 Ramachandran plot confirming that 96 % amino acids are in the allowed regions for the phi (ϕ) and psi (ψ) angles.

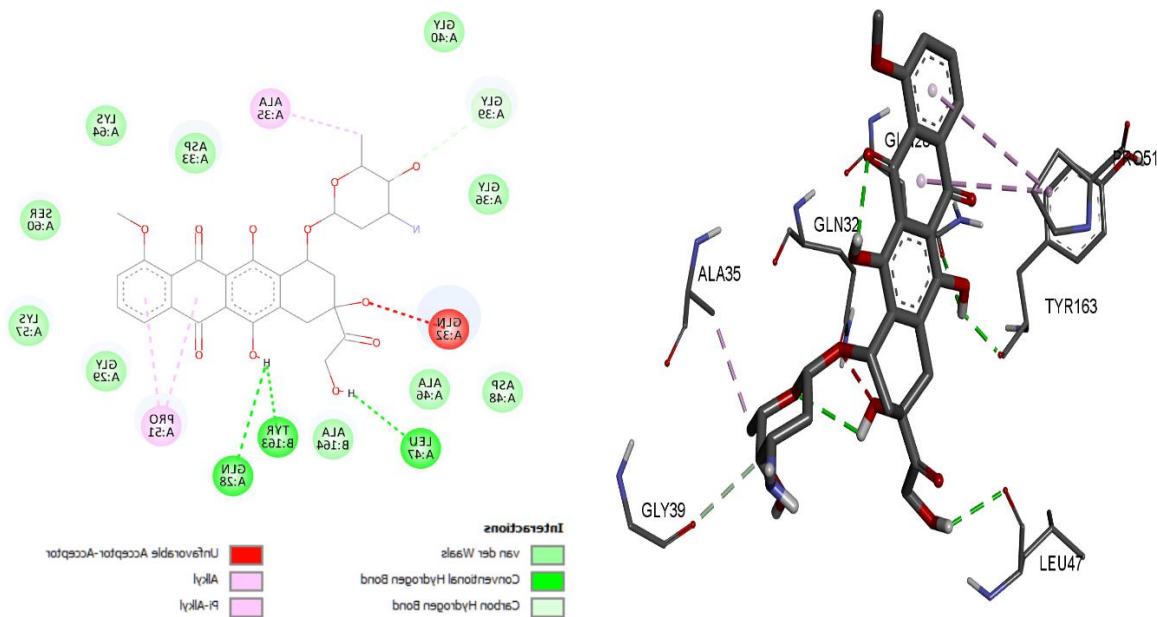


Figure S13 Representation of docked ligand with BAX (PDB-ID: 2K7W)

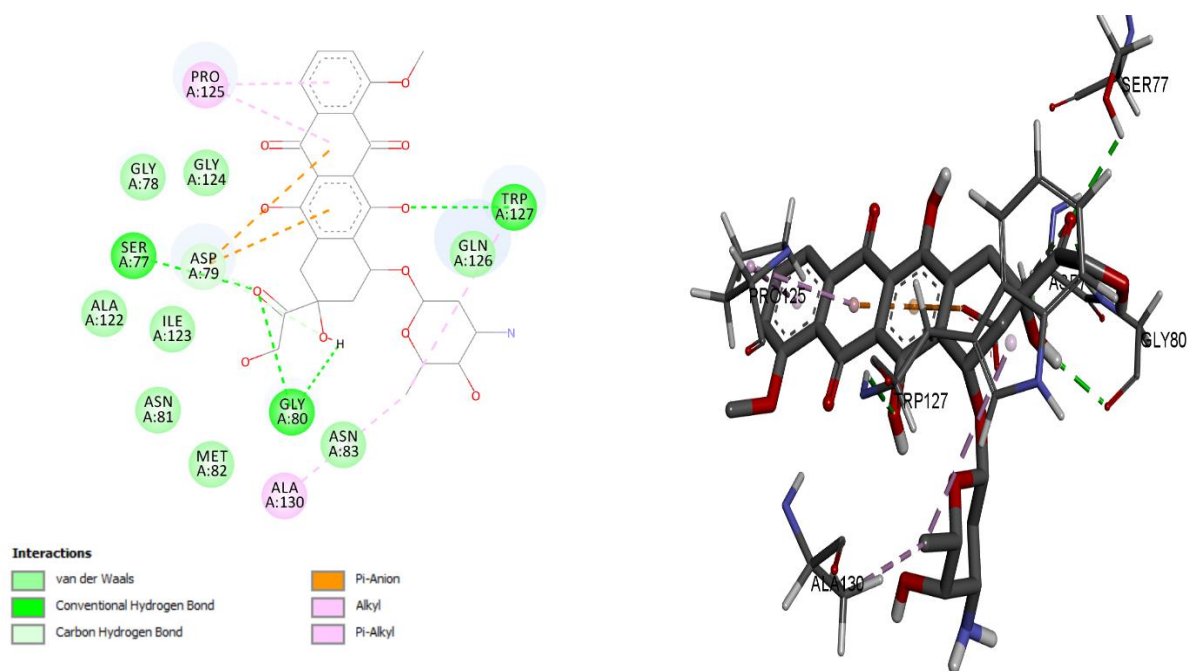


Figure S14 Representation of docked ligand with BCL-2 (PDB-ID 1K3K)

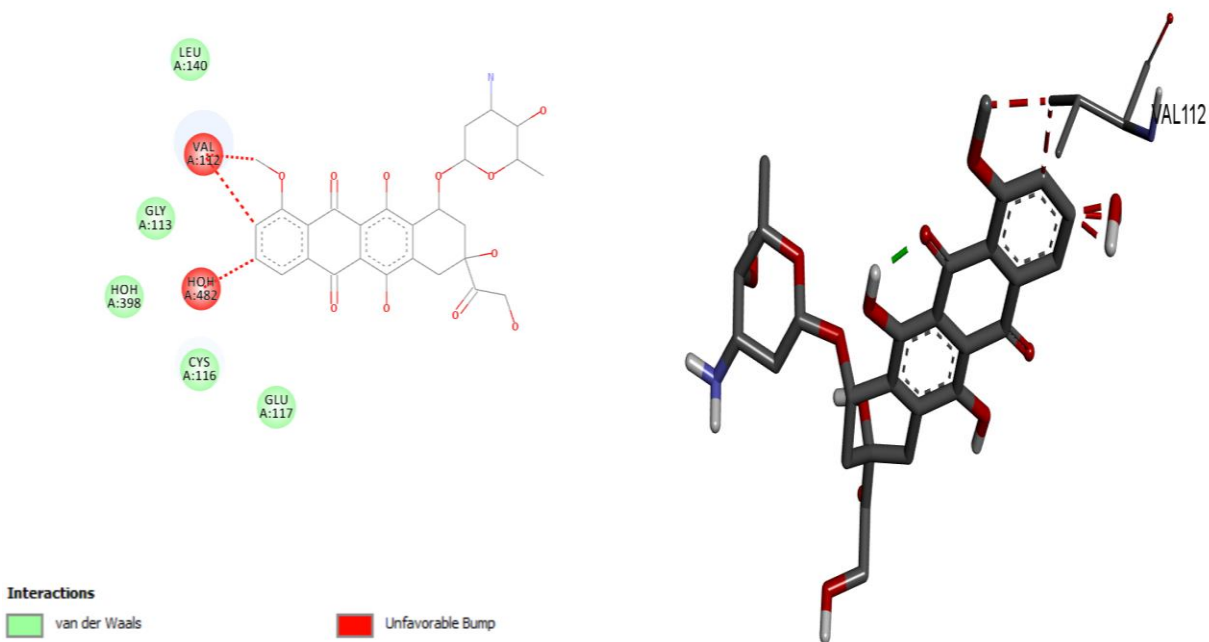


Figure S15 Representation of docked ligand with NF-kB (PDB-ID 1NFK)

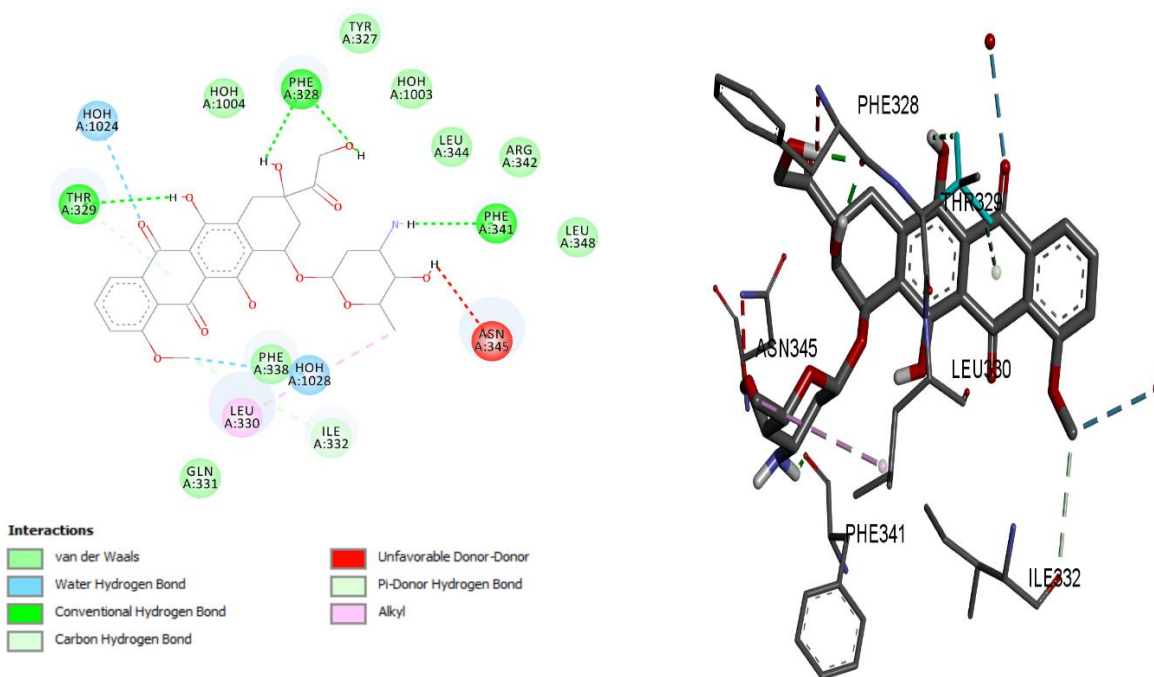


Figure S16 Representation of docked ligand with P53 (PDB-ID 1AIE)

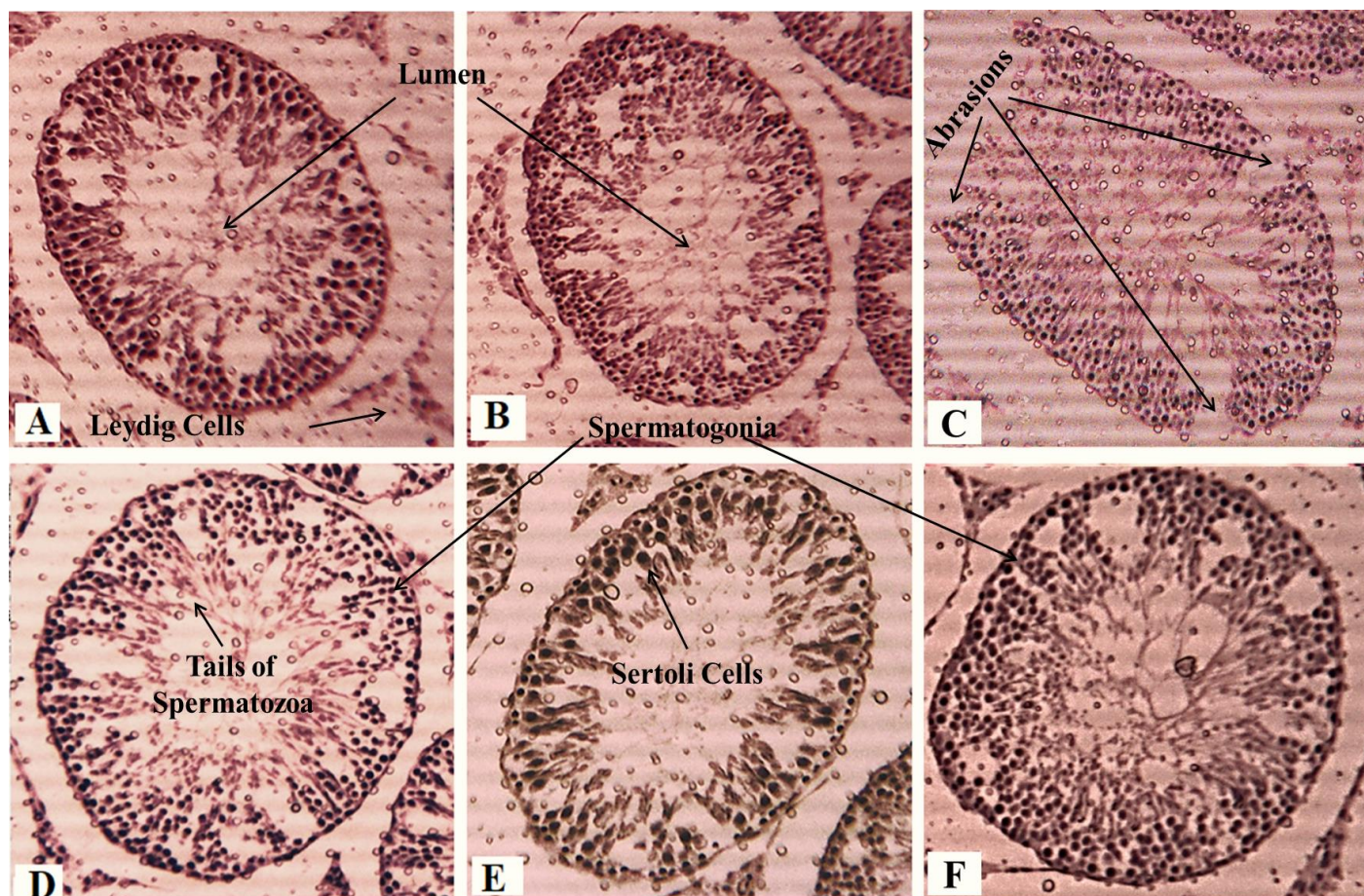


Figure S17. Histological examination for the protecting proficiency of NA on testes in rat. **Note:** 40X Hematoxylin-eosin stain. (A), Control, (B), Vehicle, (C) BPA, (D) NA (10 mg/kg), (E) BPA+NA (10 mg/kg), (F) BPA+NA (5 mg/kg).