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|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Authors** | **Regimen** | ***n*** | **Age (year)** | **CR (%)** | **2-year (3-year) EFS/PFS (%)** | **2-year (3-year) OS (%)** |
| Our current study | CHOP CVP | 251 67 | 17-82 45-87 | 69.8 29.9\* | 55.3 (46.0) 18.0 (12.0)\* | 58.0 (52.0) 25.0 (19.0)\* |
| Khaled *et al.*[1] | CHOP | 40 | 19-75 | 67 | 54 (54) | 82 (71) |
| Burton *et al.*[2] | CHOP CIOP | 105 106 | 22-66 25-67 | 70 52 | 4-year PFS: 56 4-year PFS: 40\* | 4-year OS: 65 4-year OS: 56# |

This part is footer. \**P* < 0.05, #*P* ≥ 0.05. EFS: event-free survival; PFS: progression-free survival; OS: overall survival; CHOP: cyclophosphamide, doxorubicin, vincristine, and prednisone; CVP: cyclophosphamide, vincristine, and prednisone; CIOP: cyclophosphamide, idarubicin, vincristine, and prednisone; CR: complete response. This table is cited with permission from Li *et al*.[1] published in xxx.

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|  |  |
| --- | --- |
|  | (1) |

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|  |  |
| --- | --- |
| **A** | 图二(清晰版)  **B** |
| **C** | |

**Figure 1.** We present examples of electron micrograph, non-editable and editable images in Figure 1A-C. A: description of what the Figure 1A is; B: description of what the Figure 1B is; C: description of what the Figure 1C is. This figure is quoted with permission from XX *et al*.[2]

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**Acknowledgments**

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**Authors’ contributions**

Single author:

The author contributed solely to the article.

Two or more authors:

Made substantial contributions to conception and design of the study and performed data analysis and interpretation: Salas H, Castaneda WV;

Performed data acquisition, as well as provided administrative, technical, and material support: Castillo N, Young V

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**Organization as author**

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**Conference proceedings**

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*SpectraBase*. Bio-Rad Laboratories. https://spectrabase.com/ (accessed 2020-01-05).

**Patent**

Stern, M. K.; Cheng, B. K. M. Process for preparing N-(p-nitroaryl)amides via reaction of nitrobenzene with nitriles. US 5380946, 1995.

**Preprint**

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