Electronic Supplementary Material (ESI) for Biomaterials Science.


# Electronic Supplementary Information

## Recent Progress on the Development of Near-infrared Organic Photothermal and Photodynamic Nanotherapeutics

Houjuan Zhu, Penghui Cheng, Peng Chen, and Kanyi Pu*

School of Chemical and Biomedical Engineering, Nanyang Technological University, 70 Nanyang Drive, Singapore, 637457

E-mail: kypu@ntu.edu.sg

Table 1. Summary of recent applications of NIR organic nanoparticles.

| Chromophore | Composition | NIR laser | Applications | Ref no. |
|---|---|---|---|---|
| PFTTQ | DSPE-PEG2000 | 808 nm | PTT | 78 |
| DPP and its derivative polymers | PSMA | 808 nm | PTT | 79 |
| | Liposome/PEG/curcumin | 808 nm | PA imaging, chemotherapy/PTT | 149 |
| | F127/DOX | 808 nm | Chemotherapy/PTT | 146 |
| | TPGS-CHO | 808 nm | PA imaging, chemotherapy/PTT | 150 |
| PorCP | DSPE-PEG2000-Mal | 808 nm | PTT | 80 |
| PBIBDF-BT | mPEG-b-PHEP/DOX | 808 nm | Chemotherapy/PTT | 148 |
| PPy | PVP/Fe3+; HA/DOX | 808 nm 810 nm | Chemotherapy/PTT | 151;152 |
| | PVP; SiO2 | 808 nm | PTT | 75;76 |
| | NH2-PEG-NH2/Gd-DOTA | 808 nm | MR/PA imaging/PTT | 51 |
| | PVP/PFOB | 808 nm | US imaging, PTT | 118 |
| PCB | PCB-PEG/DOX | 808 nm | NIRF, PA imaging, chemotherapy/PTT | 147 |
| oligomer N4 | DSPE-PEG2000 | 808 nm | PA imaging, PTT | 109 |
| BT/PT/DPP based polymers | DSPE-PEG2000 | 808 nm | PA imaging, PTT | 110 |
| TDI-TPA based polymer | PAA | 660 nm | PA imaging, PTT | 107 |
| TBD-based polymer | DSPE-mPEG2000 | 671 nm | PA imaging, PTT | 112 |
| DPP/thiophene based polymers | mPEG-b-PHEP | 808 nm | PA imaging, PTT | 111 |
| poly(heptamethine) | PEG−PLA | 808 nm | NIRF/PA imaging, PTT | 128 |
| Polyaniline PANI | rapamycin/DiR/DSPE-PEG2000/DPPC/FA-DSPE-PEG2000 | 808 nm | NIRF/PA imaging, chemotherapy/PTT | 126 |
| | DTPA-Gd/cetuximab/ EGFR | 808 nm | MR imaging, PTT | 125 |
| | F127; NMPA-CS | 808 nm | PTT | 74;69;73; |
| PCPDTBT | F127/PC70B | 808 nm | PA imaging, PTT | 108 |
| | F127/nanoceria; PS-PAA/$MnO_2$ /F127 | 808 nm | NIRF imaging, PDT | 162;15 |
| PDPA−PPa | OEI-C14 | 671 nm | PDT/immunotherapy | 168 |
| CPNs | DSPE-PEG2000-Mal | 808 nm | NIRF imaging, PTT/PDT | 194 |
| TBT based polymer | DSPE-mPEG2000 | 635 nm | NIRF/PA imaging PTT/PDT | 201 |
| Dpa-melanin | _ | 808 nm | MR imaging, PTT | 124 |

| CNSs | | | | |
|---|---|---|---|---|
| ICG and its derivatives | PLGA/lecithin/PEG; HAS/DOX | 808 nm | NIRF imaging chemotherapy/PTT | 140;199 |
| | PL-PEG | 808 nm | PTT; NIRF imaging, PTT | 68; 91 |
| | CS-N-Arg/DOX | 808 nm | chemotherapy/PTT | 141 |
| | epirubicin (EPI) | 808 nm | NIRF/PA imaging, chemotherapy/PTT | 87 |
| | PLGA-b-PEG/PEI; PEG-PLL-PLLeu | 808 nm | NIRF imaging, PTT | 67;92 |
| | PDA | 800 nm | PA/MR imaging, PTT | 132 |
| | holo-Tf | 808 nm | NIRF/PA imaging, PTT | 129 |
| | DSPE-PEG2000-iRGD/LPs; FDA-PEG | 808 nm | NIRF imaging, PTT/PDT | 190; |
| | HA/ MIL-100(Fe) | 808 nm | NIRF/PA/MR imaging, PTT/PDT | 133 |
| | FA/PEI-PEG-gadoteric acid/ Gd-DOTA | 808 nm | NIRF/MR imaging, PDT | 171 |
| | HSA/PTX | 808 nm | NIRF/PA imaging, PTT/PDT | 142 |
| | TPZ/PLGA/DPPC/DSPE-PEG/DSPE-PEG-DBCO | 808 nm | NIRF imaging, chemotherapy/ PDT | 178 |
| cypate | cisplatin/(P(MEO2MA-coMASI)-b-PHPMA | 805 nm | Chemotherapy/PTT | 144 |
| Cyanine | mPEG-Cy-PCL/DOX | 650 nm | NIRF imaging, chemotherapy/ PTT | 138 |
| cyanine dye RC | BSA | 915 nm | PTT | 66 |
| IR825 and its derivatives | PEG/PEI | 915 nm | PA imaging, chemotherapy/PTT | 143 |
| | PDOX | 825 nm | chemotherapy, PTT | 139 |
| | C18PMH–PEG; HSA | 808 nm | NIRF imaging, PTT | 82;83 |
| | HSA/ Cy5.5/PFOB | 808 nm | NIRF/CT imaging, PTT | 131 |
| | HSA/ DTPA-Gd | 808 nm | NIRF/MR imaging, PTT | 134 |
| | PAH/IONP/PEG; | 915 nm; | MR imaging, PTT | 114 |
| IR820 | HRGP | 808 nm | NIRF/PA imaging, PTT/PDT | 202 |
| | Docetaxel/ PCL-g-PEI | 808 nm | NIRF imaging, chemotherapy/PTT/PDT | 211 |
| IR780 and its derivatives | Heparine folic acid; lipid; PMDPC; curcumin; PEG-IR780-C13; PMPC-b-PBMA; c(RGDyK) | 808 nm | NIRF imaging, PTT | 84;85;86; 88;89;90 |
| | PPI/PCL/CPT/ RhB | 808 nm | NIRF/PA imaging chemotherapy/PTT | 137 |

| | | | | |
|---|---|---|---|---|
| | 188Re/N2H-PEG-b-PCL; Cetuximab/111In-DTPA | 808 nm | NIRF/CT/Micro-SPECT imaging, PTT | 135;136 |
| | PEG | 808 nm | NIRF/PA imaging, PTT | 127 |
| | PFTBA/HSA | 780 nm | NIRF imaging, PDT | 158 |
| | HSA; mPEG2000-SH | 808 nm | NIRF imaging, PTT/PDT | 191;192 |
| porphyrin and its derivatives | Lipid subunits | 680 nm | NIRF, PA imaging, PTT | 50 |
| | peptide | 635 nm | PA imaging, PTT | 102 |
| | PEG/GC | 635 nm | NIRF imaging, PDT | 157 |
| | Gly-Val-Arg (PLGVR) peptide | 630 nm | NIRF/AIE imaging, PDT | 163 |
| | DOX/ PVA | 690 nm | NIRF/PET imaging, chemotherapy/PTT/PDT | 210 |
| | TPZ | 660 nm | NIRF imaging, chemotherapy/PDT | 177 |
| | --- | 671 nm | PA imaging, PTT/PDT | 182 |
| IR808 | HA | 808 nm | NIRF/PA imaging, PTT | 130 |
| Ce6 and its derivatives | HA/ 5β-cholanic acid/PEG/ BHQ3; HCP/HPE; α-CD/PEG; PAMAM dendrime/RGD peptide; H-Phe-Phe-NH2·HCl | 660 nm | NIRF imaging, PDT | 155;165; 166;154; 167; |
| | HA/ADH | 660 nm | NIRF/PA imaging, PDT | 169 |
| | C18PMH-PEG-NH2/64Cu | 658 nm | NIRF/PET imaging, PDT | 164 |
| | PLGA/ HA-Gd | 670 nm | NIRF/MR imaging, PDT | 170 |
| | PDA | 660/808 nm | NIRF imaging, PTT/PDT | 187 |
| | Gd3+/DOX/PEG-b-PDPA | 655 nm | NIRF/MR/PA imaging, chemotherapy/PTT/PDT | 212 |
| | DSPE-mPEG5k/ AQ4N/64Cu | 660 nm | NIRF/PET/PA imaging, chemotherapy/PDT | 176 |
| BODIPY and its derivatives | PMAGP-POEGMA-PLys, | 721 nm | PDT | 159 |
| | PEG-PASP-DOX | 635 nm | NIRF imaging, chemotherapy/ PDT | 173 |
| | polyoxyethylene azide | 660 nm | PTT/PDT | 183 |
| | DSPE-mPEG2000 | 808 nm | PA imaging, PTT/PDT | 195 |
| croconine (Croc) | HSA | 808 nm | NIRF/PA imaging, PTT | 100 |
| croconaine rotaxane dye | POPC/CholPEG600/DOTAP | 808 nm | PA imaging, PTT | 101 |
| BBT-2FT | PEG-b-PCL | 808 nm | PA imaging, PTT | 98 |
| TPA-T-TQ | DSPE-PEG2000 | 808 nm | PA imaging, PTT | 99 |
| RET-BDP | F127-FA | 670 nm | NIRF imaging, PDT | 160 |

| | | | | |
|---|---|---|---|---|
| phthalocyanines (Pc) | PPIG4 dendrimer/PEG/LHRH | 700 nm | NIRF imaging, chemotherapy/PDT | 172 |
| SiNc | PPIG5; PEG−PCL | 785 nm | NIRF imaging, PTT/PDT | 183;193 |
| DVDMS | RGD-modified ferritin | 630 nm | NIRF/PA imaging, PTT/PDT | 206 |
| | MnO2 | 630 nm | NIRF/PA/MR imaging, PTT/PDT | 179 |
| DPP-TPA | ---- | 660 nm | PA imaging, PTT/PDT | 197 |
| Cy/Ce6 | mPEG-b-PAsp(DA) | 785/660 nm | NIRF/PA imaging, PTT/PDT | 198 |
| hCe6/DiR | DPPC/cholesterol/DSPE-mPEG5k | 785/660 nm | NIRF/PA imaging, PTT/PDT | 200 |
| Ce6/PPy | BSA/Gd | 808 nm | NIRF/MR imaging, PTT/PDT | 207 |
| Ce6/IR825 | C18PMH-PEG-Ce6-Gd | 808 nm | NIRF/MR/PA imaging, PTT/PDT | 208 |
| Pdots/Ce6 | lipid–Gd–DOTA | 670 nm | MR/PA imaging, PTT/PDT | 203 |
| TCPP/IR825 | P(PEGMA-co-APMA)-b-PMMA | 660/808 nm | NIRF/MR/PA imaging, PTT/PDT | 205 |
| IABDP | DSPE-mPEG2000 | 730 nm | PA imaging, PTT/PDT | 196 |
| PEDOT/ICG | PEG-GTA | 808/1064 nm | PTT/PDT | 185 |
| PEDOT:PSS/Ce6 | DOX/SN38/PEG | 660 nm | Chemotherapy, PTT/PDT | 209 |

Table 2. The photothermal conversion efficacy and $^1O_2$ quantum yield of NIR organic nanoparticles under NIR laser irradiation.

| NIR organic dyes or nanoparticles | photothermal conversion efficacy | $^1O_2$ quantum yield | NIR laser | Ref no. |
|---|---|---|---|---|
| Pdots (DPP based polymers) | Up to 65% | - | 808 nm | 79 |
| Porphyrin based polymer (PorCP) | 63.8% | - | 808 nm | 80 |
| Polypyrrole nanoparticles (PPy NPs) | 45% | - | 808 nm | 76 |
| PANI | 48.5% | - | 808 nm | 74 |
| poly(dopamine) (PDA) NPs | 40% | - | 808 nm | 187 |
| F127-modified PANPs (F-PANPs) | 48.5%. | - | 808 nm | 74 |
| RC-BSA nanoparticles (NPs) | 28.7% | - | 808 nm | 66 |
| IR-780-C4-curcumin assembling nanoparticles (CCNPs) | 52% | - | 808 nm | |
| Dpa-melanin CNSs | 40% | - | 808 nm | 124 |
| benzo[1,2-c;4,5-c0]bis[1,2,5]thiadiazole-4,7-bis(9,9-dioctyl-9H-fluoren-2-yl)thiophene (denoted as BBT-2FT) | 40% | - | 808 nm | 98 |
| peptide−porphyrin nanodots (PPP-NDs) | 54.2% | - | 635 nm | 102 |
| oligomer N4 NPs | 30% | - | 808 nm | 109 |
| terrylenediimide (TDI)-poly(acrylic acid) (TPA)-based nanomedicine (TNM) | 41% | - | 660 nm | 107 |
| thiophene–benzene–diketopyrrolopyrrole (TBD)-based polymer | 68.1% | - | 671 nm | 112 |
| DPP/thiophene based polymers | Up to 42.53% | - | 808 nm | 111 |
| PBIBDF-BT@NPPPE | 46.7% | - | 808 nm | 148 |
| Cur/DPP-PTSL | ~38% | - | 808 nm | 149 |
| DOX/DPP-NPs | 50% | - | 808 nm | 150 |
| DSPN5 | 30.8% | - | 808 nm | 147 |
| PEDOT/ICG | 71.1% | - | 808 nm | 185 |
| ICG | - | 0.2% | 808 nm | 15 |
| PCPDDTBT@$SiO_2$ with (SPN-M1) and without coating $MnO_2$ ((SPN-0)) | - | 7.28%, 7.64% | 808 nm | 15 |
| DPP-TPA NPs | 34.5% | 33.6% | 660 nm | 197 |
| Bodiplatin-NPs; Bodiplatin; Bodipy | 37.0%, 27.0%, 11.0% | | 660 nm | 183 |
| CPNs | 47.6% | 60.4% | 808 nm | 194 |