Takahito Nakajima

List of Publications by Year in descending order

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117 papers 3,461 citations

32 h-index 55 g-index

117 all docs

117 docs citations

117 times ranked

4263 citing authors

#	Article	lF	CITATIONS
1	Markedly Enhanced Permeability and Retention Effects Induced by Photo-immunotherapy of Tumors. ACS Nano, 2013, 7, 717-724.	7.3	237
2	The Douglas–Kroll–Hess Approach. Chemical Reviews, 2012, 112, 385-402.	23.0	197
3	Theoretical Investigation of the Excited States of Coumarin Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2007, 111, 5544-5548.	1.1	156
4	Near-infrared Theranostic Photoimmunotherapy (PIT): Repeated Exposure of Light Enhances the Effect of Immunoconjugate. Bioconjugate Chemistry, 2012, 23, 604-609.	1.8	136
5	Discovery of Pb-Free Perovskite Solar Cells via High-Throughput Simulation on the K Computer. Journal of Physical Chemistry Letters, 2017, 8, 4826-4831.	2.1	134
6	Targeted, Activatable, In Vivo Fluorescence Imaging of Prostate-Specific Membrane Antigen (PSMA) Positive Tumors Using the Quenched Humanized J591 Antibody–Indocyanine Green (ICG) Conjugate. Bioconjugate Chemistry, 2011, 22, 1700-1705.	1.8	128
7	Enhanced Catalytic Activity on Titanosilicate Molecular Sieves Controlled by Cationâ°Ï€ Interactions. Journal of the American Chemical Society, 2011, 133, 12462-12465.	6.6	96
8	Photoimmunotherapy: Comparative effectiveness of two monoclonal antibodies targeting the epidermal growth factor receptor. Molecular Oncology, 2014, 8, 620-632.	2.1	95
9	Immediate in vivo target-specific cancer cell death after near infrared photoimmunotherapy. BMC Cancer, 2012, 12, 345.	1.1	86
10	Near Infrared Photoimmunotherapy in the Treatment of Disseminated Peritoneal Ovarian Cancer. Molecular Cancer Therapeutics, 2015, 14, 141-150.	1.9	81
11	Real-time Monitoring of <i>In Vivo</i> Acute Necrotic Cancer Cell Death Induced by Near Infrared Photoimmunotherapy Using Fluorescence Lifetime Imaging. Cancer Research, 2012, 72, 4622-4628.	0.4	77
12	Improving the Efficacy of Photoimmunotherapy (PIT) using a Cocktail of Antibody Conjugates in a Multiple Antigen Tumor Model. Theranostics, 2013, 3, 357-365.	4.6	74
13	The Effect of Photoimmunotherapy Followed by Liposomal Daunorubicin in a Mixed Tumor Model: A Demonstration of the Super-Enhanced Permeability and Retention Effect after Photoimmunotherapy. Molecular Cancer Therapeutics, 2014, 13, 426-432.	1.9	61
14	In vivo breast cancer characterization imaging using two monoclonal antibodies activatably labeled with near infrared fluorophores. Breast Cancer Research, 2012, 14, R61.	2.2	60
15	Galactosyl Human Serum Albumin-NMP1 Conjugate: A Near Infrared (NIR)-Activatable Fluorescence Imaging Agent to Detect Peritoneal Ovarian Cancer Metastases. Bioconjugate Chemistry, 2012, 23, 1671-1679.	1.8	60
16	Impact of Impaired Renal Function on Gadolinium Retention After Administration of Gadolinium-Based Contrast Agents in a Mouse Model. Investigative Radiology, 2016, 51, 655-660.	3. 5	58
17	Computed tomography-guided transpulmonary radiofrequency ablation for hepatocellular carcinoma located in hepatic dome. World Journal of Gastroenterology, 2006, 12, 608.	1.4	56
18	NTChem: A highâ€performance software package for quantum molecular simulation. International Journal of Quantum Chemistry, 2015, 115, 349-359.	1.0	55

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19	Short PEG-Linkers Improve the Performance of Targeted, Activatable Monoclonal Antibody-Indocyanine Green Optical Imaging Probes. Bioconjugate Chemistry, 2013, 24, 811-816.	1.8	53
20	Photoimmunotherapy of hepatocellular carcinoma-targeting Glypican-3 combined with nanosized albumin-bound paclitaxel. Nanomedicine, 2015, 10, 1139-1147.	1.7	53
21	Detection of metastatic lesions from malignant pheochromocytoma and paraganglioma with diffusion-weighted magnetic resonance imaging: comparison with 18F-FDG positron emission tomography and 123I-MIBG scintigraphy. Annals of Nuclear Medicine, 2008, 22, 395-401.	1.2	52
22	The Effect of Perinatal Gadolinium-Based Contrast Agents on Adult Mice Behavior. Investigative Radiology, 2018, 53, 110-118.	3.5	50
23	Gadolinium MRI Contrast Agents Based on Triazine Dendrimers: Relaxivity and In Vivo Pharmacokinetics. Bioconjugate Chemistry, 2012, 23, 2291-2299.	1.8	49
24	The relativistic complete active-space second-order perturbation theory with the four-component Dirac Hamiltonian. Journal of Chemical Physics, 2006, 125, 234110.	1.2	46
25	The effects of conjugate and light dose on photo-immunotherapy induced cytotoxicity. BMC Cancer, 2014, 14, 389.	1.1	46
26	Spectroscopic and Computational Study of Acetic Acid and Its Cyclic Dimer in the Near-Infrared Region. Journal of Physical Chemistry A, 2016, 120, 6170-6183.	1.1	44
27	Comparative effectiveness of light emitting diodes (LEDs) and Lasers in near infrared photoimmunotherapy. Oncotarget, 2016, 7, 14324-14335.	0.8	42
28	Activatable Organic Near-Infrared Fluorescent Probes Based on a Bacteriochlorin Platform: Synthesis and Multicolor <i>in Vivo</i> Imaging with a Single Excitation. Bioconjugate Chemistry, 2014, 25, 362-369.	1.8	41
29	Distribution and clearance of retained gadolinium in the brain: differences between linear and macrocyclic gadolinium based contrast agents in a mouse model. British Journal of Radiology, 2016, 89, 20160509.	1.0	37
30	MPI/OpenMP Hybrid Parallel Algorithm of Resolution of Identity Second-Order Møller–Plesset Perturbation Calculation for Massively Parallel Multicore Supercomputers. Journal of Chemical Theory and Computation, 2013, 9, 5373-5380.	2.3	36
31	Minibody-Indocyanine Green Based Activatable Optical Imaging Probes: The Role of Short Polyethylene Glycol Linkers. ACS Medicinal Chemistry Letters, 2014, 5, 411-415.	1.3	35
32	Selective cell elimination in vitro and in vivo from tissues and tumors using antibodies conjugated with a near infrared phthalocyanine. RSC Advances, 2015, 5, 25105-25114.	1.7	34
33	From C ₆₀ to Infinity: Large-Scale Quantum Chemistry Calculations of the Heats of Formation of Higher Fullerenes. Journal of the American Chemical Society, 2016, 138, 1420-1429.	6.6	32
34	Preparation and long-term biodistribution studies of a PAMAM dendrimer G5–Gd-BnDOTA conjugate for lymphatic imaging. Nanomedicine, 2015, 10, 1423-1437.	1.7	31
35	Large-scale QM/MM calculations of the CaMn ₄ O ₅ cluster in the S ₃ state of the oxygen evolving complex of photosystem II. Comparison between water-inserted and no water-inserted structures. Faraday Discussions, 2017, 198, 83-106.	1.6	31
36	Acute Cytotoxic Effects of Photoimmunotherapy Assessed by ¹⁸ F-FDG PET. Journal of Nuclear Medicine, 2013, 54, 770-775.	2.8	30

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37	A dual-level approach to density-functional theory. Journal of Chemical Physics, 2006, 124, 184108.	1.2	29
38	Dielectric-dependent screened Hartree–Fock exchange potential and Slater-formula with Coulomb-hole interaction for energy band structure calculations. Journal of Chemical Physics, 2014, 141, 114109.	1.2	28
39	Theoretical modelling of biomolecular systems I. Large-scale QM/MM calculations of hydrogen-bonding networks of the oxygen evolving complex of photosystem II. Molecular Physics, 2015, 113, 359-384.	0.8	28
40	An approximate second-order Møller–Plesset perturbation approach for large molecular calculations. Chemical Physics Letters, 2006, 427, 225-229.	1.2	27
41	Role of F-18 FDG PET/CT in assessing IgG4-related disease with inflammation of head and neck glands. Annals of Nuclear Medicine, 2015, 29, 499-505.	1.2	26
42	How Can We Understand Au \cdot sub \cdot 8 \cdot sub \cdot Cores and Entangled Ligands of Selenolate- and Thiolate-Protected Gold Nanoclusters Au \cdot sub \cdot 24 \cdot sub \cdot 6ER) \cdot 8ub \cdot 20 \cdot 8ub \cdot 8 and Au \cdot 8ub \cdot 20 \cdot 8ub \cdot 9 (ER) \cdot 8ub \cdot 16 \cdot 8ub \cdot 9 (E = Se, S; R = Ph, Me)? A Theoretical Study. Journal of the American Chemical Society, 2015, 137, 8593-8602.	6.6	25
43	Effects of Gadolinium-Based Contrast Agents on Thyroid Hormone Receptor Action and Thyroid Hormone-Induced Cerebellar Purkinje Cell Morphogenesis. Frontiers in Endocrinology, 2016, 7, 115.	1.5	25
44	Two-Component Relativistic Equation-of-Motion Coupled-Cluster Methods for Excitation Energies and Ionization Potentials of Atoms and Molecules. Journal of Physical Chemistry A, 2017, 121, 827-835.	1.1	24
45	Efficient Computation of Sparse Matrix Functions for Large-Scale Electronic Structure Calculations: The <scp>CheSS</scp> Library. Journal of Chemical Theory and Computation, 2017, 13, 4684-4698.	2.3	23
46	Differentiation of sarcoidosis-lymphomaÂsyndrome lesions: a case report on the use of two different positron emission tomography tracers. BMC Medical Imaging, 2016, 16, 1.	1.4	22
47	Massively parallel algorithm and implementation of RI-MP2 energy calculation for peta-scale many-core supercomputers. Journal of Computational Chemistry, 2016, 37, 2623-2633.	1.5	22
48	Gaussian and finite-element Coulomb method for the fast evaluation of Coulomb integrals. Journal of Chemical Physics, 2007, 126, 144106.	1.2	20
49	New implementation of molecular double point-group symmetry in four-component relativistic Gaussian-type spinors. International Journal of Quantum Chemistry, 2007, 107, 1382-1389.	1.0	20
50	Evaluation of bone scan index change over time on automated calculation in bone scintigraphy. Annals of Nuclear Medicine, 2015, 29, 911-920.	1.2	20
51	Diagnostic value of 18F-fluorodeoxyglucose uptake parameters to differentiate rheumatoid arthritis from other types of arthritis. Medicine (United States), 2017, 96, e7130.	0.4	19
52	Activatable fluorescent cys-diabody conjugated with indocyanine green derivative: consideration of fluorescent catabolite kinetics on molecular imaging. Journal of Biomedical Optics, 2013, 18, 101304.	1.4	18
53	Real-time monitoring of hemodynamic changes in tumor vessels during photoimmunotherapy using optical coherence tomography. Journal of Biomedical Optics, 2014, 19, 098004.	1.4	18
54	Application of the dielectric-dependent screened exchange potential approach to organic photocell materials. Physical Chemistry Chemical Physics, 2016, 18, 27554-27563.	1.3	18

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55	Organ retention of gadolinium in mother and pup mice: effect of pregnancy and type of gadolinium-based contrast agents. Japanese Journal of Radiology, 2017, 35, 568-573.	1.0	18
56	Theoretical study on the cooperative exciton dissociation process based on dimensional and hot charge-transfer state effects in an organic photocell. Journal of Chemical Physics, 2016, 144, 234906.	1.2	17
57	Analyses of Thiophene-Based Donor–Acceptor Semiconducting Polymers toward Designing Optical and Conductive Properties: A Theoretical Perspective. Journal of Physical Chemistry C, 2016, 120, 8305-8314.	1.5	17
58	Diagnosing Ovarian Cancer on MRI: A Preliminary Study Comparing Deep Learning and Radiologist Assessments. Cancers, 2022, 14, 987.	1.7	17
59	Percutaneous radiofrequency ablation of osteoid osteoma using cool-tip electrodes without the cooling system. Japanese Journal of Radiology, 2011, 29, 138-143.	1.0	15
60	Dynamic fluorescent imaging with indocyanine green for monitoring the therapeutic effects of photoimmunotherapy. Contrast Media and Molecular Imaging, 2014, 9, 276-282.	0.4	15
61	A case of multiple hepatic angiomyolipomas with high $18\hat{a}$ %-F-fluorodeoxyglucose uptake. BMC Medical Imaging, 2014, 14, 17.	1.4	15
62	Theoretical investigation of enantioselectivity of cage-like supramolecular assembly: The insights into the shape complementarity and host-guest interaction. Journal of Computational Chemistry, 2015, 36, 459-466.	1.5	15
63	Full geometry optimizations of the CaMn4O4 model cluster for the oxygen evolving complex of photosystem II. Chemical Physics Letters, 2015, 640, 23-30.	1.2	15
64	Large-scale QM/MM calculations of the CaMn4O5 cluster in the oxygen-evolving complex of photosystem II: Comparisons with EXAFS structures. Chemical Physics Letters, 2016, 658, 354-363.	1.2	15
65	Theoretical study of exciton dissociation through hot states at donor–acceptor interface in organic photocell. Physical Chemistry Chemical Physics, 2015, 17, 12538-12544.	1.3	14
66	Full-valence density matrix renormalisation group calculations on meta-benzyne based on unrestricted natural orbitals. Revisit of seamless continuation from broken-symmetry to symmetry-adapted models for diradicals. Molecular Physics, 2017, 115, 2267-2284.	0.8	14
67	Theoretical study on the excited states of heteroarene chromophores: Comparison of calculated and experimental values. Chemical Physics Letters, 2009, 473, 196-200.	1.2	13
68	Magnetic Resonance Lymphography of the Thoracic Duct after Interstitial Injection of Gadofosveset Trisodium: A Pilot Dosing Study in a Porcine Model. Lymphatic Research and Biology, 2014, 12, 32-36.	0.5	13
69	Effects of Heteroatoms on Electronic States of Divanadium-Substituted Î ³ -Keggin-type Polyoxometalates. Inorganic Chemistry, 2014, 53, 3907-3918.	1.9	13
70	Second-order generalized unrestricted MÃ,ller–Plesset perturbation theory for the spin–orbit part of zero-field splitting tensors. Chemical Physics Letters, 2011, 515, 296-301.	1.2	12
71	The Born-Oppenheimer molecular simulations of infrared spectra of crystalline poly-(R)-3-hydroxybutyrate with analysis of weak C HâぐO C hydrogen bonds. Chemical Physics Letters, 2017, 678, 112-118.	1.2	11
72	Applying near-infrared photoimmunotherapy to B-cell lymphoma: comparative evaluation with radioimmunotherapy in tumor xenografts. Annals of Nuclear Medicine, 2017, 31, 669-677.	1.2	11

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73	Electrical anharmonicity in hydrogen bonded systems: complete interpretation of the IR spectra of the Clâ \in Hâ $_f$ stretching band in the gaseous (CH ₃) ₂ Oâ $_f$ HCl complex. Physical Chemistry Chemical Physics, 2017, 19, 5917-5931.	1.3	10
74	Shear Wave Imaging of Breast Tissue by Color Doppler Shear Wave Elastography. IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, 2017, 64, 340-348.	1.7	10
7 5	Electron-nucleus cusp correction scheme for the relativistic zeroth-order regular approximation quantum Monte Carlo method. Journal of Chemical Physics, 2010, 132, 174108.	1.2	9
76	MR lymphangiography with intradermal gadofosveset and human serum albumin in mice and primates. Journal of Magnetic Resonance Imaging, 2014, 40, 691-697.	1.9	9
77	Two-component relativistic time-dependent density functional theory study on spin-forbidden transitions for metal polypyridyl complexes. Chemical Physics Letters, 2015, 635, 152-156.	1.2	9
78	Theoretical study on spin-forbidden transitions of osmium complexes by two-component relativistic time-dependent density functional theory. Chemical Physics Letters, 2016, 648, 60-65.	1.2	9
79	An extrapolation scheme for solid-state NMR chemical shift calculations. Chemical Physics Letters, 2017, 677, 99-106.	1.2	9
80	Infrared Spectroscopy and Born–Oppenheimer Molecular Dynamics Simulation Study on Deuterium Substitution in the Crystalline Benzoic Acid. Journal of Physical Chemistry B, 2017, 121, 479-489.	1.2	9
81	A new computational scheme for the spin–orbit part of zero-field splitting tensor. Chemical Physics Letters, 2012, 549, 108-112.	1.2	8
82	SIMPLE METHOD OF SIZE-SPECIFIC DOSE ESTIMATES CALCULATION FROM PATIENT WEIGHT ON COMPUTED TOMOGRAPHY. Radiation Protection Dosimetry, 2018, 178, 208-212.	0.4	8
83	Correlation effects beyond coupled cluster singles and doubles approximation through Fock matrix dressing. Journal of Chemical Physics, 2017, 147, 204108.	1.2	7
84	Early prediction of triple negative breast cancer response to cisplatin treatment using diffusion-weighted MRI and 18F-FDG-PET. Breast Cancer, 2018, 25, 334-342.	1.3	7
85	Theoretical study of valence photoelectron spectra of Re(CO)5X (X=Cl, Br, and I): A spin-orbit DK3 symmetry-adapted cluster/symmetry-adapted cluster-configuration interaction study. Journal of Chemical Physics, 2006, 124, 224307.	1.2	6
86	Spectroscopic study of uracil, 1-methyluracil and 1-methyl-4-thiouracil: Hydrogen bond interactions in crystals and ab-initio molecular dynamics. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 197, 194-201.	2.0	6
87	Electron-Enhanced Vibrational Spectroscopy: A Theoretical Approach. Analytical Sciences, 2008, 24, 111-114.	0.8	5
88	Fluorescenceâ€ifetime molecular imaging can detect invisible peritoneal ovarian tumors in bloody ascites. Cancer Science, 2014, 105, 308-314.	1.7	5
89	Gaussian-based cutoff scheme on Hartree–Fock exchange term of dielectric-dependent potential. Chemical Physics Letters, 2015, 634, 83-87.	1.2	5
90	A case of intra-articular ganglion cysts of the knee joint: correlation between arthroscopic and magnetic resonance imaging. BMC Medical Imaging, 2016, 16, 36.	1.4	5

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91	A theoretical study on hot charge-transfer states and dimensional effects of organic photocells based on an ideal diode model. Physical Chemistry Chemical Physics, 2017, 19, 12517-12526.	1.3	5
92	18F-FDG and 18F-FAMT PET-derived metabolic parameters predict outcome of oral squamous cell carcinoma. Oral Radiology, 2019, 35, 308-314.	0.9	5
93	Texture analysis of [18F]-fluorodeoxyglucose-positron emission tomography/computed tomography for predicting the treatment response of postoperative recurrent or metastatic oral squamous cell carcinoma treated with cetuximab. Annals of Nuclear Medicine, 2021, 35, 871-880.	1.2	5
94	Quantitative analysis of metabolic parameters at 18F‑fluorodeoxyglucose positron emission tomography in predicting malignant potential of anterior mediastinal tumors. Oncology Letters, 2020, 19, 1865-1871.	0.8	5
95	The reaction of N ₂ O ₅ with H ₃ O ⁺ : A firstâ€principles direct molecular dynamics study of acidâ€catalyzed reactive uptake of N ₂ O ₅ . International Journal of Quantum Chemistry, 2009, 109, 2143-2148.	1.0	4
96	Relativistic diffusion Monte Carlo method: Zeroth-order regular approximation-diffusion Monte Carlo method in a spin-free formalism. Journal of Chemical Physics, 2012, 137, 154103.	1.2	4
97	lodine concentration calculated by dual-energy computed tomography (DECT) as a functional parameter to evaluate thyroid metabolism in patients with hyperthyroidism. BMC Medical Imaging, 2017, 17, 43.	1.4	4
98	Bioluminescence Image as a Quantitative Imaging Biomarker for Preclinical Evaluation of Cryoablation in a MurineÂModel. Journal of Vascular and Interventional Radiology, 2018, 29, 1034-1040.	0.2	4
99	Efficient evaluation of the Coulomb force in the Gaussian and finite-element Coulomb method. Journal of Chemical Physics, 2010, 132, 244107.	1.2	3
100	A dual-level approach to four-component relativistic density-functional theory. Chemical Physics Letters, 2011, 508, 177-181.	1.2	3
101	Gaussian-based range-separation approach on Hartree–Fock exchange interaction and second-order perturbation theory. Chemical Physics Letters, 2016, 647, 132-138.	1.2	3
102	A Transarterial Chemoembolization of Balloon-Occluded Alternate Infusions of Cisplatin and Gelatin Particles for Hepatocellular Carcinoma: A Phase I/II Multicenter Prospective Study of Safety and Efficacy. Journal of Vascular and Interventional Radiology, 2022, 33, 169-176.e1.	0.2	3
103	Magnetite Ingested as a Nutritional Supplement: Unexpected Source of MRI Susceptibility Artifact. American Journal of Roentgenology, 2007, 188, 1026-1027.	1.0	2
104	Advantages of L-3-[18F] fluoro-alpha-methyl tyrosine over 2-[18F]-fluoro-2-deoxyglucose in detecting liver metastasis during positron emission tomography scan. SpringerPlus, 2016, 5, 618.	1.2	2
105	UNO DMRG CASCI calculations of effective exchange integrals for m-phenylene-bis-methylene spin clusters. Molecular Physics, 2017, 115, 2154-2167.	0.8	2
106	64Cu-ATSM and 99mTc(CO)3-DCM20 potential in the early detection of rheumatoid arthritis. Modern Rheumatology, 2021, 31, 350-356.	0.9	2
107	Robust Validation and Comprehensive Analysis of a Novel Signature Derived from Crucial Metabolic Pathways of Pancreatic Ductal Adenocarcinoma. Cancers, 2022, 14, 1825.	1.7	2
108	Prefecture-wide multi-centre radiation dose survey as a useful tool for CT dose optimisation: report of Gunma radiation dose study. Radiation Protection Dosimetry, 2015, 167, 519-524.	0.4	1

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109	MPI/OpenMP hybrid parallel algorithm for resolution of identity secondâ€order Møller–Plesset perturbation calculation of analytical energy gradient for massively parallel multicore supercomputers. Journal of Computational Chemistry, 2017, 38, 489-507.	1.5	1
110	A Color-Doppler Shear-Wave-Imaging Phase-reconstruction Method Using Four Color Flow Images. Ultrasonic Imaging, 2017, 39, 172-188.	1.4	1
111	Quantum Chemical Study on the Multi-Electron Transfer of Keggin-Type Polyoxotungstate Anions: The Relation of Redox Potentials to the Bond Valence ofâ€ <i>ŵ</i> ₄ -O-W. Journal of Computer Chemistry Japan, 2017, 16, 93-95.	0.0	1
112	Activatable fluorescence detection of epidermal growth factor receptor positive mediastinal lymph nodes in murine lung cancer model. PLoS ONE, 2018, 13, e0198224.	1.1	1
113	Abstract 5400: Photoimmunotherapy (PIT) combined with a nanosized cancer agent successfully treated heterogenous antigen-expressing tumors based on super-enhanced permeability and retention (SUPR) effect., 2014,,.		1
114	Relation between Wavelength Dispersion of Refractive Index and Birefringence of Polymers Estimated by Quantum Chemical Calculation and Chemical Structure. Kobunshi Ronbunshu, 2009, 66, 119-129.	0.2	0
115	Abstract LB-508: A GSA-NMP1 conjugate: An NIR-activatable fluorescence imaging agent to detect peritoneal ovarian cancer metastases. , 2012, , .		0
116	Abstract 4830: Target-molecular specific near infrared cancer photoimmunotherapy: Detection, treatment, and monitoring of tumors with a theranostic fluorescent probe. , 2012, , .		0
117	Abstract 4512: Super-enhanced permeability and retention (SUPR) effect induced by photo-immunotherapy (PIT) can accommodate massive nano-sized reagents deep into tumors, 2013,,.		O