core PFOB
Perfluorooctylbromide
Component of nanoparticle core
PubChem CID: 9873
Canonical SMILES C(C(C(C(C(F)(F)Br)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F

core PFDCO
Perfluorodichlorooctane
Component of nanoparticle core
PubChem CID: 2774033
Canonical SMILES: C(C(C(C(C(F)(F)Cl)(F)F)(F)F)(F)F)(C(C(C(F)(F)Cl)(F)F)(F)F)(F)F

DOPC
1,2-Dioleoyl-sn-Glycero-3-Phosphocholine
PubChem CID 10350317
Canonical SMILES CCCCCCCCC=CCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCC=CCCCCCCCC

DPPC
1,2-Dipalmitoyl-sn-glycero-3-phosphocholine
PubChem CID 3032281
Canonical SMILES CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCC

core PFO
Perflurooctane
Component of nanoparticle core
PubChem CID: 9387
Canonical SMILES: C(C(C(C(C(F)(F)F)(F)F)(F)F)(F)F)(C(C(C(F)(F)F)(F)F)(F)F)(F)F

core PFC
Perfluoro-15-crown-5 ether 96%(wt/vol)
Component of nanoparticle core
PubChem CID 2776038
Canonical SMILES: C1(C(OC(C(OC(C(OC(C(OC(C(O1)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F)(F)F

core Safflower Oil
Component of nanoparticle core x(wt/vol)
PubChem SID 53789663

PubChem CID: 13183956
Canonical SMILES
CCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CCCCCCCC=CCCCCCCCC

Isomeric SMILES
CCCCCCCCCCCCCCCCCC(=O)OCC(COC(=O)CCCCCCCCCCCCCCCCC)OC(=O)CCCCCCC\\C=C/
CCCCCCCC

safflower oil
PubChem SID SID: 53789663

Indium Acetate
PubChem CID 168292
Canonical SMILES: CC(=O)[O-].CC(=O)[O-].CC(=O)[O-].[In+3]

excipient Glycerin
Humectant
Component of emulsion excipient 2.3 %(wt/vol) Ralph Fuhrhop
 PubChem CID: 753
Canonical SMILES: C(C(CO)O)O

coating Lipid Layer
Lipid surfactant comixture 2%(wt/vol)

coating Lecithin
Phosphatidylcholine
 Component of lipid layer
 Pubmed CID: 24798685
Canonical SMILES: C[N+](C)(C)CCOP(=O)(O)OCC(COC=O)OC=O
Isomeric SMILES: C[N+](C)(C)CCOP(=O)(O)OC[C@@H](COC=O)OC=O

1-octadecene
PubChem CID 8217
Canonical SMILES: CCCCCCCCCCCCCCCCC=C

N-Boc-ethylenediamine
PubChem CID 187201
Canonical SMILES : CC(C)(C)OC(=O)NCCN

sulfuric acid
PubChem CID 1118
Canonical SMILES : OS(=O)(=O)O

methanol
PubChem CID: 887
Canonical SMILES: CO

Carbon Tetrabromide
PubChem CID 11205
Canonical SMILES: C(Br)(Br)(Br)Br

Monomethoxypolyethylene Glycol
Poly-(Ethylene Glycol) Methyl Ether
5000 Da

PubChem SID 24852066
Canonical SMILES: C(CO)O

HEPES
4-(2-Hydroxyethyl)-1-piperazineethanesulfonic acid
PubChem CID 23831
Canonical SMILES : C1CN(CCN1CCO)CCS(=O)(=O)O

coating Cholesterol
Description Cholest-5-en-3-ol 8 mole%
Component of lipid layer
PubChem CID: 638019
Canonical SMILES: CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C
Isomeric SMILES: CC(C)CCC[C@@H](C)
[C@@H]1CC[C@H]2[C@]1(CC[C@@H]3[C@@H]2CC=C4[C@@]3(CC[C@@

Alexa Fluor 488-NHS
Fluorophore activated with N-hydroxysuccinimide ester moiety

NaCL
sodium chloride
PubChem CID 5234
Canonical SMILES : [Na+].[Cl-]

modification PE
Phosphatidylethanolamine 1.8 mole%
Component of lipid layer
MW: 271.161721 g/mol | MF: C7H14NO8P   PubChem CID: 24771772
Canonical SMILES: C(COP(=O)(O)OCC(COC=O)OC=O)N

nickel acetate
PubChem CID 9756
Canonical SMILES : CC(=O)[O-].CC(=O)[O-].[Ni+2]

Diarsenic trioxide
PubChem CID 261004
Canonical SMILES : O=[As]O[As]=O

NIPAAM
N-isopropylacrylamide (SigmaAldrich)
PubChem CID 16637
Canonical SMILES : CC(C)NC(=O)C=C

VP
1-Vinyl-2-pyrrolidone (SigmaAldrich)
PubChem CID 6917

DVB
divinyl benzene
crosslinker

PubChem CID 66666
Canonical SMILES : C=CC1=CC=CC=C1C=C

AA
acrylic acid   (SigmaAldrich)
PubChem CID 6917
Canonical SMILES : C=CC(=O)O

N,N'-Methylenebis(acrylamide)
 N,N'-methylene-bis-acrylamide
PubChem CID 8041
Canonical SMILES : C=CC(=O)NCNC(=O)C=C

ferrous sulfate
CID 24393
Canonical SMILES : [O-]S(=O)(=O)[O-].[Fe+2]

ferrous ferric oxide
PubChem ID   6432052
Canonical SMILES : [O-2].[O-2].[O-2].[O-2].[Fe+2].[Fe+3].[Fe+3]

TEMED
N,N,N',N'-tetramethylethylenediamine
PubChem CID 8037
Canonical SMILES : CN(C)CCN(C)C

curcumin

PubChem CID 969516
Canonical SMILES :
COC1=C(C=CC(=C1)C=CC(=O)CC(=O)C=CC2=CC(=C(C=C2)O)OC)O

pyridine
PubChem CID 1049
Canonical SMILES C1=CC=NC=C1

acetic anhydride
PubChem CID 7918
Canonical SMILES CC(=O)OC(=O)C

Biotin Cap DPPE
Biotin-cap-dipalmitoyl-phosphotidylethanolamine
1,2-Dipalmitoyl-sn-Glycero-3-Phosphoethanolamine-N-(Cap Biotinyl)
Component of lipid layer
Avidin targeting agent
MW 1,052.659 MF C53H98N4O11PNaS
http://www.avantilipids.com/ProductData.asp?n=870277

DPPE

1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine (Avanti Polar Lipids 850705)
PubChem CID 445468
Canonical SMILES : CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)(O)OCCN)OC(=O)CCCCCCCCCCCCCCC

modification DPPE
Dipalmitoyl Phosphatidylethanolamine 0.1 mole%
Bidentate ligand
Component of lipid layer
PubChem CID: 65109
Canonical SMILES: CCCCCCCCCCCCCCCC(=O)OCC(COP(=O)(O)OCCN)OC(=O)CCCCCCCCCCCCCCC

PEG
Polyethylene glycol - hydrophilic polymer with antibiofouling properties
MW: 634.751120 g/mol | MF: C28H58O15 PubChem CID: 656926?????????
Canonical SMILES: C(COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)O ???

modificattion   Peptidomimetic Vitronectin Receptor Antagonist
Peptidomimetic vitronectin receptor antagonist conjugated to (PEG)2000-phosphatidylethanolamine
Alpha-nu-beta-3 integrin targeting agent.
Component of lipid layer
Inherent function
targeting
Targeting alpha-nu-beta-3 integrins - cell adhesion receptors involved in cell-extracellular matrix and cell-cell interactions

FA
Description Folic Acid
PubChem   CID: 6037
Canonical SMILES:
C1=CC(=CC=C1C(=O)NC(CCC(=O)O)C(=O)O)NCC2=CN=C3C(=N2)C(=O)N=C(N3)N
Inherent Function targeting
Targeting folate receptors in KB cells
Glycosylphosphatidylinositol (GPI)-linked membrane glycoprotein overexpressed
in variety of tumors

Methanol
PubChem CID 887
Canonical SMILES: CO

Ethanol
PubChem CID 702
Canonical SMILES: CCO

mPEG-Amine

amine terminated monomethoxy Poly(Ethylene) Glycol

modification Rhodamine PE
  Rhodamine phosphatidylethanolamine 0.1 mole%
 Fluorescent dye and phosphatidylethanolamine conjugate
Component of lipid layer

Rhodamine B
Fluorone dye
MW: 479.010340 g/mol | MF: C28H31ClN2O PubChem CID: 6694
Canonical SMILES: CCN(CC)C1=CC2=C(C=C1)C(=C3C=CC(=[N+]
(CC)CC)C=C3O2)C4=CC=CC=C4C(=O)O.[Cl-]

Rhodamine
5-carboxytetramethylrhodamine Fluorone dye
PubChem CID 2762602
Canonical SMILES: CN(C)C1=CC2=C(C=C1)C(=C3C=CC(=[N+]
(C)C)C=C3O2)C4=C(C=C(C=C4)C(=O)[O-])C(=O)O

DMF
N,N-dimethylformamide
polar (hydrophilic) aprotic solvent
PubChem CID 6228
Canonical SMILES: CN(C)C=O

herceptin
PubChem SID 17397410

oxalyl chloride
PubChem CID 65578
Canonical SMILES : C(=O)(C(=O)Cl)Cl

Pyropheophorbide a
3(1),3(2)-didehydrophytochlorin
Photosensitizer
PubChem CID: 5489042
Canonical SMILES:
CCC1=C2C=C3C(=C4C(=O)CC(=C5C(C(C(=N5)C=C6C(=C(C(=CC(=C1C)N2)N6)C=C)C)C
)CCC(=O)O)C4=N3)C

Octane-1,8-Diol
1,8-Octanediol
PubChem CID 69420
Canonical SMILES: C(CCCCO)CCCO

N-(3-Dimethylaminopropyl)-N-Ethylcarbodiimide
ChemSpider ID: 10630780
SMILES: CC[N](=C=N)CCCN(C)C

DTPA
Diethylene Triamine Pentaacetic Acid
Chelate
PubChem CID 3053
Canonical SMILES: C(CN(CC(=O)O)CC(=O)O)N(CCN(CC(=O)O)CC(=O)O)CC(=O)O

NHS-PEG-MAL
N-hydroxysuccinimide Poly(Ethylene-Glycol) Maleimide
Heterobifunctional crosslinker

NHS-PEG
N-hydroxysuccinimide Poly(Ethylene Glycol)

modification Gd-DTPA-BOA
Gadolinium-diethylene-triamine-pentaacetic-acid-bis-oleate 30 mole%
Complex of chelate and imaging contrast agent
Component of lipid layer
MF C50H90N5O8Gd Grace Hu
C(CN(CCN(CCN(CC(=O)N([H])CCCCCCC\C(=C([H])/CCCCCCCO[H])[H])CC(=O)
[O-])CC(=O)[O-])CC(=O)[O-])(N([H])CCCCCCCC(=C([H])CCCCCCCO[H])[H])=O.
[Gd+]
molecular structure
Patrick Winter, Phillip Athey, Garry Kiefer, Gyongyi Gulyas, Keith
Frank,
Ralph Fuhrhop, David Robertson, Samuel Wickline, Gregory Lanza
Journal of Magnetism and Magnetic Materials 293 (2005) 540–545   doi:
10.1016/j.jmmm.2005.01.062
Inherent function
Imaging   MRI
MRI imaging of artherosclerosis induced angiogenesis in animal model

modification Gd-DTPA-PE
Description Gadolinium-diethylene-triamine-pentaacetic-acid-
phosphatidylethanolamine 30 mole%
Complex of chelate and imaging contrast agent
Component of lipid layer
Inherent Function imaging MRI
 MRI imaging of fibrin plasma clots and ex vivo human carotid artery

modification Fumagillin
Chemotherapeutic drug – naturally secreted antibiotic from Aspergillus
fumigatus
  Component of lipid layer
PubChem CID: 5351474
  Canonical SMILES: CC(=CCC1C(O1)
(C)C2C(C(CCC23CO3)OC(=O)C=CC=CC=CC(=O)O)OC)C
Isomeric SMILES: CC(=CCC1C(O1)(C)C2C(C(CCC23CO3)OC(=O)\\C=C\\C=C\\C=C\
\C=C/C(=O)O)OC)C
Inherent function therapeutic

Inhibitor of angiogenic endothelial cells proliferation by inhibiting activity of methionine aminopeptidase 2 (MetAP2) enzyme.

modification Biotin
Cofactor involved in metabolism of fatty acids
MW: 244.310640 g/mol | MF: C10H16N2O3S PubChem CID: 171548
Canonical SMILES: C1C2C(C(S1)CCCCC(=O)O)NC(=O)N2
Isomeric SMILES: C1[C@H]2[C@@H]([C@@H](S1)CCCCC(=O)O)NC(=O)N2

modification Biotinylated PE
1,2-Dihexadecanoyl-sn-Glycero-3-Phosphoethanolamine-N-(Biotinyl)
Component of lipid layer
MF C47H87N3O10PNaS MW 940.236
Avanti Polar Lipids 870285
Inherent Function Targeting
Targeting porcine plasma combined with thrombin, exposed to excess biotinylated anti-fibrin antibody, and treated with avidin

modification Biotin Cap DPPE
Description Biotin-cap-dipalmitoyl-phosphotidylethanolamine 2 mole%
Component of lipid layer.
Avidin targeting agent.
1,2-Dipalmitoyl-sn-Glycero-3-Phosphoethanolamine-N-(Cap Biotinyl)
MW 1,052.659 MF C53H98N4O11PNaS
http://www.avantilipids.com/ProductData.asp?n=870277
Inherent Function targeting
Targeting human fibrin plasma clots and ex vivo human carotid artery treated with biotinylated antifibrin monoclonal antibodies and avidin.

MPB-PE
1,2-Dipalmitoyl-sn-Glycero-3-Phosphoethanolamine-N-4-(p-Maleimidophenyl) Butyramide
Functionalized lipid
MF C51H84N2O11PNa
MW 955.183
http://www.avantilipids.com/index.php?option=com_content&view=article&id=771&Itemid=183&catnumber=870013

SH-PEG-COOH
heterofunctional PEG

H2O
water
PubChem CID: 962
Canonical SMILES O

potassium carbonate
PubChem CID: 11430
Canonical SMILES C(=O)([O-])[O-].[K+].[K+]

sodium citrate
PubChem CID: 6224
Canonical SMILES C(C(=O)[O-])C(CC(=O)[O-])(C(=O)[O-])O.[Na+].[Na+].[Na
+]

sodium citrate tribasic
trisodium citrate dihydrate
PubChem CID 71474
Canonical SMILES C(C(=O)[O-])C(CC(=O)[O-])(C(=O)[O-])O.O.O.[Na+].[Na
+].[Na+]

hydroquinone
reducing agent
PubChem CID: 785
Canonical SMILES C1=CC(=CC=C1O)O

chloroauric acid
PubChem CID: 28133
Canonical SMILES [H+].Cl[Au-](Cl)(Cl)Cl

formaldehyde
PubChem CID: 712
Canonical SMILES C=O

THPC
tetrakis(hydroxymethyl) phosphonium chloride
PubChem CID: 31298
Canonical SMILES C(O)[P+](CO)(CO)CO.[Cl-]

carbon monoxide
PubChem CID: 281
Canonical SMILES [C-]#[O+]

mPEG-SH
Methoxy-PEG-Thiol
CH3O(CH2CH2O)nCH2CH2SH
stabilizing PEG

mPEG-NH2

mPEG-SMB
alpha-methyl-PEG-succinimidyl alpha-methylbutanoate

MAL-PEG-NHS
maleimide-PEG-N-hydroxysuccinimide

APS-3
3-aminopropyltrimethoxysilane
PubChem CID 83756

Canonical SMILES: CO[Si](CCCN)(OC)OC

APTES
3-aminopropyltriethoxysilane
PubChem CID: 13521
Canonical SMILES CCO[Si](CCCN)(OCC)OCC

BTEOSE
1,2-bis(triethoxysilyl)ethane
PubChem CID 85266
Canonical SMILES: CCO[Si](CC[Si](OCC)(OCC)OCC)(OCC)OCC

THPMP
3-trihydroxysilyl)propyl methylphosphonate
PubChem CID 4385787
Canonical SMILES: CP(=O)([O-])OCCC[Si](O)(O)O.[Na+]

Chlorauric Acid
Gold Tetrachloride Acid
PubChem CID 28133
Canonical SMILES: [H+].Cl[Au-](Cl)(Cl)Cl

DY776-NHS
DY776-N-succinimidyl ester
NHS modified fluorophore
PubChem CID 10463539
Canonical SMILES: CC[N
+]1=C2C=C3C(=C(C=C(O3)C4=CC=CC=C4)C=CC=CC=C5C(C6=C(N5CCCS(=O)(=O)
[O-])C=CC(=C6)S(=O)(=O)[O-])
(C)CCCC(=O)ON7C(=O)CCC7=O)C=C2C(=CC1(C)C)C.[Na+]

DY776 silane precursor
SMILES [C][C]O[Si]([C][C][C][N]C(=O)[C][C][C]C5([C])C(=[C][C]=[C]
[C]=[C]C1=[C]C(=[O+]C2=[C]C3=C([C]=C12)C(
=[C]C([C])([C])N3[C][C])[C])C4=[C][C]=[C][C]=[C]4)N([C][C][C][S]([O-])
([O-])[O-])C6=C5[C]=C([C]=[C]
6)[S]([O-])([O-])[O-])(O[C][C])O[C][C].[Na+]

chloramine-T
PubChem CID 3641960
Canonical SMILES: CC1=CC=C(C=C1)S(=O)(=O)[N-]Cl.[Na+]

THPAL
trialanine phosphine
SMILES CC(NCP(CNC(C)C(=O)O)CNC(C)C(=O)O)C(=O)O from Vijaya Kattumuri
thesis
ChemSpider ID: 8462144
SMILES: O=C(O)C(NCP(CNC(C(=O)O)C)CNC(C(=O)O)C)C

Sodium Tetrachloroaurate
PubChem CID 27127
Canonical SMILES: [Na+].Cl[Au-](Cl)(Cl)Cl

Gum Arabic
polysaccharides and glycoprotein complex
PubChem SID 167362

Maltose
dextrodisaccharide from malt and starch
PubChem CID 6255
Canonical SMILES: C(C1C(C(C(C(O1)OC2C(OC(C(C2O)O)O)CO)O)O)O)O

Sodium Hydroxide
Caustic metallic base
PubChem CID 14798
Canonical SMILES: [OH-].[Na+]

Avanti Polar Lipids 870277
16:0 Biotinyl Cap PE
1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine-N-(cap biotinyl)
(sodium salt)
[H][C@@](COC(=O)CCCCCCCCCCCCCCC)(COP(=O)
([O-])OCCNC(=O)CCCC[C@@]2([H])SC[C@@]1([H])NC(=O)N[C@]12[H])OC(=O)CCCC
CCCCCCCCCCC Molinspiration WebMe Editor no sodium

output from PubChem sketcher after entering output from
Molinspiration
[C@@H]([C]OC(=O)[C][C][C][C][C][C][C][C][C][C][C][C][C][C][C])([C]O[P]
(=O)([O-])O[C][C][N]C(=O)[C][C][C][C][C@H]1S[C][C@H]2[N]C(=O)[N]
[C@@H]12)OC(=O)[C][C][C][C][C][C][C][C][C][C][C][C][C][C][C]

phenyl boronic acid
PubChem CID 66827
Canonical SMILES : B(C1=CC=CC=C1)(O)O

3-carboxyphenylboronic acid
PubChem CID 2733957
Canonical SMILES : B(C1=CC(=CC=C1)C(=O)O)(O)O

modification MGITC
Description Malachite Green Isothiocyanate - near-infrared Raman
reporter
Molecular Formula: C24H24ClN3O4S
Molecular Weight: 485.98
CAS Number/Name: 147492-82-8
Methanaminium, N-[4-[[4-(dimethylamino)phenyl](4-
isothiocyanatophenyl)methylene]-2,5- cyclohexadien-1-ylidene]-N-
methyl-, chloride

http://probes.com/servlets/structure?item=689
http://www.analytchem.tugraz.at/fluorophores/Show_SearchResult.php?Spacer=0&Substance_ID=699&Application=1
[C]1=C([C]=[C]C(=[C]1)C(=C2[C]=[C]C([C]=[C]2)=[N+](C([H])([H])[H])C([H])([H])[H])C3=[C][C]=C([C]=[C]3)N=C=S)N(C([H])([H])[H])C([H])([H])[H].[Cl](=O)(=O)(=O)[O-]

modification DTTC
Description Diethylthiatricarbocyanine iodide - ultraviolet Raman reporter
15,300 crystal violet molecules per gold particle
MW: 544.513870 g/mol | MF: C25H25IN2S2 PubChem CID: 5702699
Canonical SMILES: CCN1C2=CC=CC=C2SC1=CC=CC=CC3=[N+](C4=CC=CC=C4S3)CC.[I-]
Isomeric SMILES: CCN\1C2=CC=CC=C2S/C1=C\C=C\C=C\C=C\C3=[N+](C4=CC=CC=C4S3)CC.[I-]

modification COOH
hydroxycarbonyl
PubChem CID: 5460610
Canonical SMILES: [C](=O)O

Et3N
triethylamine
PubChem CID: 8471
Canonical SMILES CCN(CC)CC

anhydrous dimethyl sulfoxide
PubChem CID 679
Canonical SMILES : CS(=O)C

coat EDC
1-Ethyl-3-[3-Dimethylamino-propyl]Carbodiimide Hydrochloride
Zero-length heterobifunctional crosslinker
zero-length Crosslinker couples carboxyl groups to primary amines
http://www.piercenet.com/Objects/View.cfm?type=ProductFamily&ID=02030312
PubChem CID: 2723939
Canonical SMILES   CCN=C=NCCCN(C)C.Cl

coat EDC
Ethyldimethylaminopropyl Carbodiimide
Zero-length heterobifunctional crosslinker
PubChem CID 15908
Canonical SMILES: CCN=C=NCCCN(C)C

PBS
phosphate buffered saline
PubChem CID 24978514

Canonical SMILES OP(=O)(O)[O-].OP(=O)([O-])[O-].[Na+].[Na+].[Na+].
[Cl-].[Cl-].[K+].[K+]

DMAP
4-Dimethylaminopyridine
PubChem CID 14284
Canonical SMILES: CN(C)C1=CC=NC=C1

2-Bromoisobutyryl Bromide
PubChem CID 88685
Canonical SMILES: CC(C)(C(=O)Br)Br

t-BA
tetrabutylammonium
PubChem CID 16028
Canonical SMILES: CCCC[N+](CCCC)(CCCC)CCCC

Ammonium Hydroxide
PubChem CID 14923
Canonical SMILES: [NH4+].[OH-]

Cu(I)Br
Copper(I) Bromide
PubChem CID 24593
Canonical SMILES: [Cu]Br

N-(3-Dimethylaminopropyl)-N'-Ethylcarbodiimide
Carbodiimide crosslinking reagent
PubChem CID 15908
Canonical SMILES: CCN=C=NCCCN(C)C

Folic acid - N-[p-[[(2-amino-4-hydroxy-6-pteridinyl) methyl]-
amino]benzoyl]-L-glutamic acid,
B complex vitamin
PubMed CID: 6037
Canonical SMILES:
C1=CC(=CC=C1C(=O)NC(CCC(=O)O)C(=O)O)NCC2=CN=C3C(=N2)C(=O)N=C(N3)N
Inherent Function targeting
Description Targeting folate receptor
Glycosylphosphatidylinositol (GPI)-linked membrane glycoprotein
overexpressed
in variety of tumors

PGA
Poly-l-glutamic acid (PGA) sodium salt (Mw = 15,000~50,000)
Sigma-Aldrich   P4761
Poly(Glutamic Acid)
PubChem CID: 33032
Canonical SMILES: C(CC(=O)O)C(C(=O)O)N

NaBH4
Sodium Borohydride
Reducing agent
PubChem CID: 4311764
Canonical SMILES: [BH4-].[Na+]

AuCl3
gold chloride auric chloride
PubChem CID 26030
Canonical SMILES : Cl[Au](Cl)Cl

SHPP
N-succinimidyl-3-[4-hydroxyphenyl]propionate
Bolton-Hunter reagent
PubChem CID: 99557
Canonical SMILES: C1CC(=O)N(C1=O)OC(=O)CCC2=CC=C(C=C2)O

1,4-dioxane
dehydrating agent
PubChem CID 31275
Canonical SMILES: C1COCCO1

Sodium Chloride
PubChem CID 5234
Canonical SMILES: [Na+].[Cl-]

coat sulfo-NHS
N-hydroxysulfosuccinimide
Crosslinking reagent
PubChem CID: 23697313
Canonical SMILES: C1C(C(=O)N(C1=O)O)S(=O)(=O)[O-].O.[Na+]

coat GMBS Heterobifunctional crosslinker
4-maleimidobutyric acid N-hydroxysuccinimide ester
PubChem CID: 133440
Canonical SMILES: C1CC(=O)N(C1=O)OC(=O)CCCN2C(=O)C=CC2=O

coat SATA Heterobifunctional crosslinker
S-Acetylthioglycolic Acid N-hydroxysuccinimide Ester
PubChem CID: 127532
Canonical SMILES: CC(=O)SCC(=O)ON1C(=O)CCC1=O
Canonical SMILES: C(C(=O)O)S

coat Sulfo-LC-SPDP
Sulfosuccinimidyl 6-(3'-[2-pyridyldithio]-propionamido)hexanoate
Heterobifunctional, thiol-cleavable and membrane permeable crosslinker
http://www.piercenet.com/Products/Browse.cfm?fldID=02030365
PubChem CID: 4588467
Canonical SMILES:

C1C(C(=O)N(C1=O)OC(=O)CCCCCNC(=O)CCSSC2=CC=CC=N2)S(=O)(=O)[O-].[Na+]

coat sulfo-SMCC (sulfosuccinimidyl4-(N-maleimidomethyl)cyclohexane-1-carboxylate
Heterobifunctional, water-soluble, non-cleavable and membrane impermeable crosslinker
http://www.piercenet.com/products/browse.cfm?fldID=02030378
PubChem CID: 16219679
Canonical SMILES: C1CC(CCC1CN2C(=O)C=CC2=O)C(=O)ON3C(=O)CC(C3=O)S(=O)(=O)O.[Na]

Sulfo-LC-SMPT
Sulfosuccinimidyl 6-[alpha-Methyl-alpha-(2-Pyridyldithio)Toluamido]Hexanoate
Water-soluble heterobifunctional crosslinker
MW:603.67 MF: C24H26N3NaO8S3
http://www.piercenet.com/Products/Browse.cfm?fldID=02030382
C1=NC(=CC=C1)SSC(C2=CC=C(C=C2)C(=O)N(CCCCCC(=O)ON3C(CC(C3=O)[S](=O)(=O)[O-])=O)[H])C.[Na+] PubChem Sketcher

 LC-SMCC
Description Succinimidyl-4-[N-Maleimidomethyl]cyclohexane-1-carboxy-[6-amidocaproate]
Heterobifunctional crosslinker, with an extended spacer arm
O=C(CCCCCNC(=O)C2CCC(CN1C(=O)CCC1=O)CC2)ON3C(=O)CCC3=O PubChem Sketcher

Hydroxylamine Hydrochloride
PubChem CID 21645
Canonical SMILES: [NH3+]O.[Cl-]

Ferric chloride hexahydrate
PubChem CID: 16211236
Canonical SMILES: O.O.O.O.O.O.Cl[Fe](Cl)Cl

Ferrous chloride tetrahydrate
PubChem CID: 16211588
Canonical SMILES: O.O.O.O.Cl[Fe]Cl

Iron Sulfate Heptahydrate
Iron(2+) Sulfate Heptahydrate
PubChem CID 62662
Canonical SMILES: O.O.O.O.O.O.O.[O-]S(=O)(=O)[O-].[Fe+2]

Ferric Nitrate Nonahydrate
Iron[III] Nitrate
PubChem CID 16211566
Canonical SMILES: [N+](=O)([O-])[O-].[N+](=O)([O-])[O-].[N+](=O)([O-])[O-].O.O.O.O.O.O.O.O.O.[Fe+3]

Iron Oxide
Superparamagnetic monocrystalline core Fe3O4
PubChem CID 6432052
Canonical SMILES: [O-2].[O-2].[O-2].[O-2].[Fe+2].[Fe+3].[Fe+3]

Chemspider ID: 4937312
Chemspider SMILES: [Fe+2].[Fe+3].[Fe+3].[O-2].[O-2].[O-2].[O-2]

64Cu Radioisotope
PET imaging agent 3.7 MBq

Copper Chloride
PubChem CID 169664
PET imaging agent
Canonical SMILES: [Cl-].[Cl-].[Cu+2]

SPDP
Description 500-fold excess N-succinimidyl 3-(2-pyridyldithio)propionate
Heterobifunctional crosslinking reagent with amine and sulfhydryl reactivity
PubChem CID 100682
Canonical SMILES: C1CC(=O)N(C1=O)OC(=O)CCSSC2=CC=CC=N2

SPDP-dPEP12-NHS ester
http://www.quantabiodesign.com/shop/item.aspx?itemid=208
heterobifunctional pegylation crosslinker reagent with amine and sulfhydryl/thiol reactivity
C1=CC=CC(=N1)SSCCC(=O)N(CCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(=O)ON2C(CCC2=O)=O)[H] PubChem Sketcher
O=C(CCSSc1ccccn1)NCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCC(=O)ON2C(=O)CCC2=O JME

CPT
Camptothecin
PubChem CID: 24360
Canonical SMILES: CCC1(C2=C(COC1=O)C(=O)N3CC4=CC5=CC=CC=C5N=C4C3=C2)O
lambda_ex 370 nm, lambda_em 440 nm
Inherent Function therapeutic
Description Inhibits DNA topoisomerase I enzyme by binding to topo I and DNA
complex, stabilizing it, which is leading to DNA damage and apoptosis.
Inherent Function imaging fluorescent

DOTAP
1,2-Dioleoyloxy-3-(trimethylammonium)propane
PubChem CID: 6437371
Canonical SMILES CCCCCCCCC=CCCCCCCCC(=O)OCC(C[N+](C)

(C)C)OC(=O)CCCCCCCC=CCCCCCCCC

DOPE
Dioleoylphosphatidylethanolamine
PubChem CID: 6437392
Canonical SMILES CCCCCCCCC=CCCCCCCCC(=O)OCC(COP(=O)(O)OCCN)OC(=O)CCCCCCCC=CCCCCCCCC

HDA
n-Hexadecylamine
PubChem CID 8926
Canonical SMILES : CCCCCCCCCCCCCCCCN

TOPO
PubChem CID 65577
Canonical SMILES : CCCCCCCCP(=O)(CCCCCCCC)CCCCCCCC

MAA
Mercaptoacetic acid - solubilizing agent allowing covalent protein attachment
MW: 92.116960 g/mol | MF: C2H4O2S PubChem CID: 1133
Canonical SMILES: C(C(=O)O)S

Acetic Anhydride
Acetyl acetate
PubChem CID: 7918
Canonical SMILES: CC(=O)OC(=O)C

coating Chemical Name EDTA
Chelator 10 mM
Ethylenediamine tetraacetic acid
MW: 292.242640 g/mol | MF: C10H16N2O8 PubChem CID: 6049
Canonical SMILES: C(CN(CC(=O)O)CC(=O)O)N(CC(=O)O)CC(=O)O

S-(2-Pyridyldithio) Cysteamine Hydrochloride
PubChem CID 13985234
Canonical SMILES: C1=CC=NC(=C1)SSCCN.Cl
Chemspider ID 10718221
SMILES: Cl.NCCSSc1ccccn1

coating Chemical Name TCEP
Tris(2-carboxyethyl) phosphine hydrochloride
Reducing agent
MW: 286.646501 g/mol | MF: C9H16ClO6P PubChem CID: 2734570
Canonical SMILES: C(CP(CCC(=O)O)CCC(=O)O)C(=O)O.Cl

modification Hydroxycarbonyl
 Carboxyl group
MW: 45.017440 g/mol | MF: CHO2 PubChem CID: 5460610

Canonical SMILES: [C](=O)O

modification DOTA
1,4,7,10-tetraazacyclododecane- 1,4,7,10-tetraacetic acid
Chelating agent
PubChem CID: 10549615
Canonical SMILES: C1CN(CCN(CCN(CCN1CC(=O)O)CC(=O)O)CC(=O)O)CC(=O)O

modification DOTA-SCN

Maleimido-mono-amide-DOTA
 1,4,7,10-Tetraazacyclododecane-1,4,7-Tris-acetic acid-10-
maleimidoethylacetamide
Bifunctional ligand
http://www.macrocyclics.com/cgi-bin/content2/ishopper/ishopper.cgi?
mode=listcat&catId=44
O=C(O)CN2CCN(CC(=O)O)CCN(CC(=O)NCCn1c(=O)ccc1=O)CCN(CC(=O)O)CC2 JME
C1CN(CCN(CCN(CCN1CC(=O)O)CC(=O)O)CC(=O)O)CC(=O)N([H])CCN2C(C=CC2=O)=O
PubChem Sketcher

amine-reactive benzyl
isothiocyante derivative of 1,4,7,10-tetraazacyclododecane-
1,4,7,10-tetraacetic acid

modification DOTA-NCS
DOTA derivative

Acetic Anhydride
Acetyl acetate
PubChem CID: 7918
Canonical SMILES: CC(=O)OC(=O)C

Biotin-X-X-NHS
Description Biotinylation reagent 0.5 mg/mL
biotinamidohexanoyl-6-amino-hexanoic acid N-hydroxy-succinimide ester
http://www.sigmaaldrich.com/catalog/search/ProductDetail/SIGMA/B3295
MW: 567.698040 g/mol | MF: C26H41N5O7S PubChem CID: 16219024
Canonical SMILES:
C1CC(=O)N(C1=O)OC(=O)CCCCCNC(=O)CCCCCNC(=O)CCCCC2C3C(CS2)NC(=O)N3

Epichlorohydrin
Crosslinker
PubChem CID 7835
Canonical SMILES: C1C(O1)CCl

crosslinked dextran
Polidexide sulfate
    MW: 1757.052680 g/mol | MF: C75H147N6O37S-   PubChem CID: 3085263

Canonical SMILES: CCN(CC)CC[N+](CC)
(CC)CCOC1C(C(C(OC1OCC2C(C(C(C(O2)OCC3C(C(C(C(O3)O)O)O)O)OCC(COC4C(OC(C(C
4O)OCCN(CC)CC)O)COC5C(C(C(C(O5)COC6C(C(C(C(O6)CO)OCCN
(CC)CC)O)O)OCCN(CC)CC)O)OCCN(CC)CC)O)O)O)O)CO)O)O.[O-]S(=O)(=O)
[O-]
Isomeric SMILES: CCN(CC)CC[N+](CC)(CC)CCO[C@@H]1[C@H]([C@@H]([C@H]
(O[C@@H]1OC[C@@H]2[C@H]
([C@@H]([C@H]([C@H](O2)OC[C@@H]3[C@H]([C@@H]([C@H]([C@H]
(O3)O)O)O)O)OCC(CO
[C@@H]4[C@H](O[C@@H]([C@@H]([C@H]4O)OCCN(CC)CC)O)CO[C@@H]5[C@@H]
([C@H](
[C@@H]([C@H](O5)CO[C@@H]6[C@@H]([C@H]([C@@H]([C@H]
(O6)CO)OCCN(CC)CC)O)O)
OCCN(CC)CC)O)OCCN(CC)CC)O)O)O)O)CO)O)O.[O-]S(=O)(=O)[O-]

dextran
polysaccharide
MW: 504.437080 g/mol | MF: C18H32O16 PubChem CID: 5460037
Canonical SMILES:
C(C1C(C(C(C(O1)OCC2C(C(C(C(O2)OCC(C(C(C(C=O)O)O)O)O)O)O)O)O)O)O)O
Isomeric SMILES: C([C@@H]1[C@H]([C@@H]([C@H]([C@H](O1)OC[C@@H]2[C@H]
([C@@H]([C@H]([C@H]
(O2)OC[C@H]([C@H]([C@@H]([C@H](C=O)O)O)O)O)O)O)O)O)O)O)O

Dextran
Polysaccharide
PubChem SID 7847128

gp100 A peptide vaccine consisting of the amino acids 280 through 288 of the melanoma antigen
glycoprotein 100 (gp100) with potential antineoplastic activity. gp100:280-288(288V) peptide
has a valine substitution at amino acid position 288 to improve immunogenicity. Vaccination
with gp100:280-288(288V) peptide may stimulate the host immune system to mount a cytotoxic
T lymphocyte (CTL) response against tumor cells positive for the gp100 antigen, resulting
in decreased tumor growth

DEAE-Dextran
Diethylaminoethyl-Dextran - Polycationic derivative of Dextran
http://pkcas.dk/204-147-___diethylaminoethyl-dextran.htm

SIY
synthetic peptide SIYRYYGL
cross-reacts with 2C TCR in complex with H-2Kb
Regulated Expression of a Tumor-Associated Antigen
Reveals Multiple Levels of T-Cell Tolerance in a

Mouse Model of Lung Cancer
Cheung, Ann F. and Dupage, Michel J P. and Dong, H Katie and Chen, Jianzhu and Jacks, Tyler
Cancer Res 68

(SIA); (Molbio Ultra, 99+%)
Succinimidyl iodoacetate
[39028-27-8]; C6H6NO4I; Mr=283.02; mp 148 C
Spacer Arm length: 1.5
http://www.molbio.com/Heterobi.htm
1. Eur. J. Biochem. (1984) 140, 63.
2. Rector, E.S., Schwenk, R.J., Tse, K.S., Sehon, A., Chan, H. (1978) J. Immun. Meth. 24, 321.
2. Wunderbaldinger, P.; Josephson, L.; Weissleder, R. (2002) Bioconjugate Chem. 13, 264-268.

glycidyl ether
PubChem CID 16704
Canonical SMILES C1C(O1)COCC2CO2

Poly(Ethylene Glycol) Monomethylether Monomethacrylate
   MW 1,000 g/mol)
   Hydrophilic macromonomers used to introduce hydrophilic sites into polymers,
   to stabilize polymer emulsions, and in synthesis of comb polymers. (n) value is MW of pEO unit
   H2C=C(CH3)CO2(CH2CH2O)nCH
   CAS Number: 26915-72-0

AEMHCl
    2-aminoethylmethacrylate hydrochloride (AEMHCl),
   Used for preparation of polymers containing primary amine groups
   and preparation of specialty methacrylate monomers.
   PubChem CID 75495
   Canonical SMILES: CC(=C)C(=O)OCCN.Cl

fluorescein-O-acrylate
    Fluorescent Monomer
   PubChem CID 5072272
   Canonical SMILES:
C=CC(=O)OC1=CC2=C(C=C1)C3(C4=C(O2)C=C(C=C4)O)C5=CC=CC=C5C(=O)O3

tert-Butyl Acrylate
PubChem CID 15458
Canonical SMILES: CC(C)(C)OC(=O)C=C

AIBN
2,2'-Azobis(isobutyronitrile)
PubChem CID 6547

Canonical SMILES: CC(C)(C#N)N=NC(C)(C)C#N

DDMAT
S-1-dodecyl-S'-(alpha,alpha'-dimethyl-alpha"-acetic acid)trithiocarbonate
Chain Transfer Agent

Styrene
PubChem CID 7501
Canonical SMILES: C=CC1=CC=CC=C1

TFA
Trifluoroacetic Acid
PubChem CID 6422
Canonical SMILES: C(=O)(C(F)(F)F)O

dichloromethane
PubChem CID 6344
Canonical SMILES : C(Cl)Cl

2,2-diethoxyacetophenone
1 wt%
Photocuring agent
PubChem CID: 22555
Canonical SMILES: CCOC(C(=O)C1=CC=CC=C1)OCC

2-(2-Chloroethoxy)-Ethanol
Canonical SMILES: C(COCCCl)O
PubChem CID 12361

Rhodamine
Fluorone dye
5-carboxytetramethylrhodamine
Molecular Formula: C25H22N2O5
Molecular Weight: 430.46
CAS Number/Name: 91809-66-4
http://probes.invitrogen.com/media/msds/06121.html
http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/22575

Rhodamine B
fluorone dye
PubChem CID 6694
Canonical SMILES : CCN(CC)C1=CC2=C(C=C1)C(=C3C=CC(=[N+](CC)CC)C=C3O2)C4=CC=CC=C4C(=O)O.[Cl-]

(2-Hydroxypropyl)-beta-cyclodextrin
PubChem CID 4581822
Canonical SMILES :

CC(COCC1C2C(C(C(O1)OC3C(OC(C(C3OCC(C)O)OCC(C)O)OC4C(OC(C(C4OCC(C)O)OCC
(C)O)OC5C(OC(C(C5OCC(C)O)OCC(C)O)OC6C(OC(C(C6OCC(C)O)OCC(C)O)OC7C(OC(C
(C7OCC(C)O)OCC(C)O)OC8C(OC(O2)C(C8OCC(C)O)OCC(C)O)COCC(C)O)COCC(C)O)CO
CC
(C)O)COCC(C)O)COCC(C)O)COCC(C)O)OCC(C)O)OCC(C)O)O

beta-cyclodextrins
PubChem CID CID 24238
Canonical SMILES : Canonical SMILES :
C(C1C2C(C(C(O1)OC3C(OC(C(C3O)O)OC4C(OC(C(C4O)O)OC5C(OC(C(C5O)O)OC6C(OC
(C(C6O)O)OC7C(OC(C(C7O)O)OC8C(OC(O2)C(C8O)O)CO)CO)CO)CO)CO)CO)O)O)O

(2-Hydroxypropyl)-beta-cyclodextrin
PubChem CID 4581822
Canonical SMILES :
CC(COCC1C2C(C(C(O1)OC3C(OC(C(C3OCC(C)O)OCC(C)O)OC4C(OC(C(C4OCC(C)O)OCC
(C)O)OC5C(OC(C(C5OCC(C)O)OCC(C)O)OC6C(OC(C(C6OCC(C)O)OCC(C)O)OC7C(OC(C
(C7OCC(C)O)OCC(C)O)OC8C(OC(O2)C(C8OCC(C)O)OCC(C)O)COCC(C)O)COCC(C)O)CO
CC
(C)O)COCC(C)O)COCC(C)O)COCC(C)O)OCC(C)O)OCC(C)O)O

2-aminoethyl methacrylate
CID 75496
Canonical SMILES : CC(=C)C(=O)OCCN

SB505124
2-(5-benzo(1,3)dioxol-5-yl-2-tert-butyl-3H-imidazol-4-yl)-6-
methylpyridine hydrochloride hydrate
transforming growth factor-beta inhibitor
PubChem CID 9858940
Canonical SMILES : CC1=CC=CC(=N1)C2=C(N=C(N2)C(C)
(C)C)C3=CC4=C(C=C3)OCO4
therapeutic
inhibits selectively transforming growth factor-beta Type I receptors
ALK4, ALK5, and ALK7

hexanol
PubChem CID 8103
Canonical SMILES : CCCCCCO
organic alcohol dehydrator

IL-2 interleukin-2
secreted cytokine regulating proliferation T and B lymphocytes
induces or expands activation of melanoma-specific T-cell responses.

Protamine #1 PRRRR SSSRP VRRRR RPRVS RRRRRRRGGR RRR (22R's of 32) MW
4252.1
Reynolds et al, http://dx.doi.org/10.1021/bc050145   Table 1.

Protamine #2 PRRRR SSSRP IRRRR PRRAS RRRRR RGGRR RR (22R's of 32)

4237.5
Reynolds et al, http://dx.doi.org/10.1021/bc050145   Table 1.

Protamine #3 Composition not known MW 4321.5
 Reynolds et al, http://dx.doi.org/10.1021/bc050145   Table 1.

Protamine #4 Composition not known MW 4065.5
Reynolds et al, http://dx.doi.org/10.1021/bc050145   Table 1.
Arginine rich peptide with the ability to translocate through cell membranes
 and accumulate in the nucleus.
 Futaki S http://dx.doi.org/10.1074/jbc.M007540200
 Inherent Function other .
    Cellular membrane translocation

PEG (C2 H4 O)n H2 O CAS Registry Number: 25322-68-3 SciFinder

PEG Molecular Formula H(OCH2CH2)nOH CAS Number 25322-68-3
Sigma-Aldrich 81150 Poly(ethylene glycol)

1,2-ethanediol; glycol; ETHYLENE GLYCOL
  MW: 62.067840 g/mol | MF: C2H6O2 PubChem CID: 174

PEG
  Polyethylene glycol - hydrophilic polymer with antibiofouling properties
  MW: 634.751120 g/mol | MF: C28H58O15 PubChem CID: 656926
Canonical SMILES: C(COCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)O

EDAC/EDC
1-ethyl-3-(3-dimethylaminopropyl) carbodiimide
zero-length crosslinking agent
PubChem CID 15908
Canonical SMILES : CCN=C=NCCCN(C)C

nano gamma-Fe2O3
iron(III) oxide
PubChem CID 518696
Canonical SMILES : O=[Fe]O[Fe]=O

phycoerythrin phylloerythrin PE
PubChem CID: 5480977
Canonical SMILES
CCC1=C(C2=CC3=C(C(=C(N3)C=C4C(=C(C(=N4)C5=C6C(=C(C(=N6)C=C1N2)C)C(=O)C5)CCC(=O)O)C)C)CC)

Polyethyleneimine   PEI
PubChem SID 134991395

EDAC/EDCI

1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride
zero-length crosslinking agent
PubChem CID 2723939
Canonical SMILES : CCN=C=NCCCN(C)C.Cl

PEO-PCL
Description Poly(ethylene oxide)-modified poly(epsilon-caprolactone) -
biodegradable polymer

PEI
Description branched polyethylenimine
Organic strongly cationic polymer that binds to certain proteins
PubChem SID 24865591 25 kDa
PubChem CID: 9033
0.1%
Canonical SMILES: C1CN1
Inherent Function other
Enables cell penetration through rapid endocytosis

Type modification Chemical Name BTDA
Description 3,3',4,4'-Benzophenone tetracarboxylic dianhydride
Aromatic dianhydride
MW: 322.225340 g/mol | MF: C17H6O7 PubChem CID: 75498
Canonical SMILES:
C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O

Arabinogalactan polysaccharide
MW: 500.491440 g/mol | MF: C20H36O14 PubChem CID: 24847856
Canonical SMILES:
CC1C(C(C(C(O1)CO)O)OC2C(C(C(C(O2)COC3C(C(C(CO3)O)OC)O)O)OC)O)O

PVA
Poly(vinyl alcohol)
MW: 44.052560 g/mol | MF: C2H4O PubChem CID: 11199
Canonical SMILES: C=CO

PEO-PCL
Description Poly(ethylene oxide)-modified poly(epsilon-caprolactone)

THF
tetrahydrofuran
PubChem CID: 8028
Canonical SMILES: C1CCOC1

trisphosgene
PubChem CID: 94429
Canonical SMILES C(=O)(OC(Cl)(Cl)Cl)OC(Cl)(Cl)Cl

Phe

L-phenylalanine (SigmaAldrich)
PubChem CID: 6140
Canonical SMILES C1=CC=C(C=C1)CC(C(=O)O)N

PCL
Poly(epsilon-caprolactone)
Monomer
PubChem CID 10401
Canonical SMILES: C1CCC(=O)OCC1

111InCl3
Indium(I) chloride
PubChem CID 6452255
Canonical SMILES: [Cl-].[Cl-].[Cl-].[In+3]

Ammonium Acetate
PubChem CID 517165
Canonical SMILES: CC(=O)[O-].[NH4+]

TOAB
Description Tetra-n-octylammonium Bromide
PubChem CID: 2734117

DDA
Description Dodecylamine
PubChem CID: 13583

Pc 4
Description Silicon phthalocyanine 4
Photosensitizing Agent
PubChem CID: 119185
Canonical SMILES: CN(C)CCC[Si](C)(C)
[O-].C1=CC=C2C(=C1)C3=CC4=NC(=NC5=C6C=CC=CC6=C([N-]5)

Ferric Chloride Hexahydrate
PubChem CID 16211236
Canonical SMILES: O.O.O.O.O.O.Cl[Fe](Cl)Cl

Ferrous Chloride Tetrahydrate
PubChem CID 16211588
Canonical SMILES: O.O.O.O.Cl[Fe]Cl

CL
epsilon-Caprolactone
PubChem CID 10401
Canonical SMILES: C1CCC(=O)OCC1
Polycaprolactone - a biodegradable thermoplastic polymer

5-Fu
5-Fluorouracil
Chemotherapeutic antimetabolite drug - inhibits thymidylate synthase (TS) and
incorporation of its metabolites into RNA and DNA
PubChem CID: 3385
Canonical SMILES: C1=C(C(=O)NC(=O)N1)F

sodium pertechnate Tc 99m
PubChem CID 23689036
Canonical SMILES : [O-][Tc](=O)(=O)=O.[Na+]

hydrochloric acid
PubChem CID: 313
Canonical SMILES Cl

ammonium sulfate
PubChem CID: 6097028
Canonical SMILES [NH4+].[NH4+].[O-]S(=O)(=O)[O-]

drug Doxorubicin
Chemotherapeutic drug - intercalates with DNA inducing single and double-strand
breaks in DNA interfering with DNA replication and RNA synthesis.
MW: 543.519260 g/mol | MF: C27H29NO11 PubChem CID: 31703
Canonical SMILES:
CC1C(C(CC(O1)OC2CC(CC3=C(C4=C(C(=C23)O)C(=O)C5=C(C4=O)C=CC=C5OC)O)(C(=O)
CO)O)N)O
Isomeric SMILES: C[C@H]1[C@H]([C@H](C[C@@H](O1)O[C@H]2C[C@@](CC3=C(C4=C(C(=C23)O)C(=O)C5=
C(C4=O)C=CC=C5OC)O)(C(=O)CO)O)N)O

Inhibits RNA and DNA replication by inhibiting unwinding DNA via interference
with the function of enzymes involved in DNA replication

drug Docetaxel
Chemotherapeutic drug - inhibits mitosis by shifting the dynamic equilibrium between tubulin dimers and
microtubules toward polymerization, thereby stabilizing microtubules.
MW: 807.879220 g/mol | MF: C43H53NO14 PubChem CID: 148124
Canonical SMILES: CC1=C2C(C(=O)C3(C(CC4C(C3C(C(C2(C)C)(CC1OC(=O)C(C(C5=CC=CC=C5)NC(=O)OC(C)(C)C)O)O)OC(=O)C6=CC=CC=C6)(CO4)OC(=O)C)O)C)O
Isomeric SMILES: CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@H]4[C@]([C@H]3[C@@H]([C@@](C2(C)C)(C
[C@@H]1OC(=O)[C@@H]([C@H](C5=CC=CC=C5)NC(=O)OC(C)(C)C)O)O)OC(=O)C6=CC=CC=C6)(CO4)OC(=O)C)O)C)O

paclitaxel/taxol
Description Chemotherapeutic agent
PubChem CID: 36314
Canonical SMILES: CC1=C2C(C(=O)C3(C(CC4C(C3C(C(C2(C)C)
(CC1OC(=O)C(C(C5=CC=CC=C5)NC(=O)C6=CC=CC=C6)O)O)OC(=O)C7=CC=CC=C7)
(CO4)OC(=O)C)O)C)OC(=O)C
Isomeric SMILES: CC1=C2[C@H](C(=O)[C@@]3([C@H](C[C@@H]4[C@]
([C@H]3[C@@H]([C@@](C2(C)C)(C
[C@@H]1OC(=O)[C@@H]([C@H]
(C5=CC=CC=C5)NC(=O)C6=CC=CC=C6)O)O)OC(=O)C7=CC=
CC=C7)(CO4)OC(=O)C)O)C)OC(=O)C

Function therapeutic
Stabilizes microtubules in their polymerized form leading to cell death

Succinic Anhydride
PubChem CID 7922
Canonical SMILES: C1CC(=O)OC1=O

DCM
dichloromethane
Methylene Chloride
PubChem CID 6344
Canonical SMILES: C(Cl)Cl

DMAP
4-dimethylaminopyridine
PubChem CID 14284
Canonical SMILES: CN(C)C1=CC=NC=C1

Pluronic F-108
 Nonionic polyoxyethylene-polyoxypropylene block co-polymer
PubChem CID 24751
Canonical SMILES: CC1CO1.C1CO1

cholesterol
PubChem CID: 5997
Canonical SMILES CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)O)C)C

Rhodamine-Paclitaxel
Chemotherapeutic drug labeled with fluorescent dye

tamoxifen
Description Chemotherapeutic drug - selective estrogen receptor modulator with tissue-specific activities
 and angiogenic inhibitor; GCS inhibitor; enzyme glucosylceramide synthase (GCS)

MW: 371.514560 g/mol | MF: C26H29NO PubChem CID: 5376
Canonical SMILES: CCC(=C(C1=CC=CC=C1)C2=CC=C(C=C2)OCCN(C)C)C3=CC=CC=C3

verapamil
Description Calcium ion influx inhibitor; moodulates the influx of ionic calcium across the cell membrane of
the arterial smooth muscle as well as in conductile and contractile myocardial cells;
Inhibitor of P-glycoprotein efflux pump contributing to drug resistance
MW: 454.601620 g/mol | MF: C27H38N2O PubChem   CID: 2520
Canonical SMILES: CC(C)C(CCCN(C)CCC1=CC(=C(C=C1)OC)OC)
(C#N)C2=CC(=C(C=C2)OC)OC

C2 Ceramide N-acetyl sphingosine   N-acetylsphingosine
PubChem CID 5497136
Canonical SMILES: CCCCCCCCCCCCCC=CC(C(CO)NC(=O)C)O

C10 Ceramide N-decanoyl-D-erythro-sphingosine N-[(E,2S,3R)-1,3-dihydroxyoctadec-4-en-2-yl]decanamide
PubChem CID 5702615
Canonical SMILES: CCCCCCCCCCCCCC=CC(C(CO)NC(=O)CCCCCCCCC)O

C14 Ceramide N-myristoyl-D-erythro-sphingosine N-(1,3-dihydroxyoctadec-4-en-2-yl)tetradecanamide
PubChem CID 5176144
Canonical SMILES: CCCCCCCCCCCCCC=CC(C(CO)NC(=O)CCCCCCCCCCCCC)O

C18 Ceramide N-stearoyl-D-erythro-sphingosine
PubChem CID 6372196
Canonical SMILES: CCCCCCCCCCCCCCCCCC(=O)NC(CO)C(C=CCCCCCCCCCCCCC)O

C24 Ceramide N-lignoceroyl-D-erythro-sphingosine
PubChem CID 5789754
Canonical SMILES:
CCCCCCCCCCCCCCCCCCCCCCCC(=O)NC(CO)C(C=CCCCCCCCCCCCCC)O

C6 Ceramide - sphingolipid produced in response to diverse stimuli which include
 growth factor deprivation, cytokines, ionizing radiation, heat shock, chemotherapy,
 is involved in cell signaling which contributes to cell cycle arrest, terminal
 cell differentiation, apoptosis, and cell proliferation
Description Second messenger in the apoptotic signaling cascade produced in response
to various stimuli, involved in cell signaling contributing to cell cycle arrest, terminal
cell differentiation, apoptosis, and cell proliferation

MW: 397.634880 g/mol | MF: C24H47NO3 PubChem CID: 16219484
Canonical SMILES: CCCCCCCCCCCCCC=CC(C(CO)NC(=O)CCCCC)O
Inherent Function therapeutic
Description Enhances Paclitaxel therapeutic effects

C6 Ceramide
Sphingolipid produced in response to diverse stimuli
Second messenger in the apoptotic signaling cascade
PubChem CID: 16219484
Canonical SMILES: CCCCCCCCCCCCCC=CC(C(CO)NC(=O)CCCCC)O
Inherent Function therapeutic
Descrption Enhances Paclitaxel therapeutic effects

NBD
Fluorophore
PubChem CID 445938
Canonical SMILES: C1=CC=C(C=C1)CNC2=NC=NC3=C2N=CN3C4C(C(C(O4)COP(=O)(O)OP(=O)(O)OCC5C(C(C(O5)[N+]6=CC=CC(=C6)C(=O)N)O)O)O)O

NBD-ceramide
Fluorescent ceramide
MW: 575.739960 g/mol | MF: C30H49N5O6 PubChem CID: 6379314
Canonical SMILES:
CCCCCCCCCCCCCC=CC(C(CO)NC(=O)CCCCCNC1=CC=C(C2=NON=C12)[N+](=O)[O-])O
Isomeric SMILES: CCCCCCCCCCCCC\C=C
\C(C(CO)NC(=O)CCCCCNC1=CC=C(C2=NON=C12)[N+](=O)[O-])O
NBD-cholesterol

NBD-cholesterol - Green fluorescent dye cholesterol conjugate
(22-(N-(7-nitrobenz-2-oxa-1,3-diazol-4-yl)amino)-23,24-bisnor-5-cholen-3-beta-ol) cholesterol
PubChem CID: 127604
Canonical SMILES: CC(CNC1=CC=C(C2=NON=C12)[N+](=O)[O-])C3CCC4C3(CCC5C4CC=C6C5(CCC(C6)O)C)C

polygalacturonic acid

Polygalacturonic Acid
Description Galacturonic acid 600 mg
MW: 194.139400 g/mol | MF: C6H10O7 PubChem CID: 84740
Canonical SMILES: C(=O)C(C(C(C(C(=O)O)O)O)O)O

galacturonate
MW: 194.139400 g/mol | MF: C6H10O7 PubChem CID: 445929
Canonical SMILES: C1(C(C(OC(C1O)O)C(=O)O)O)O
Isomeric SMILES: [C@@H]1([C@H]([C@H](O[C@@H]([C@@H]1O)O)C(=O)O)O)O

Acetic Anhydride
Acetyl acetate
PubChem CID: 7918

Canonical SMILES: CC(=O)OC(=O)C

Succinyl-(2-Hydroxypropyl)-beta-cyclodextrin
SigmaAldrich S0565

NEt3
Triethylamine
chemical intermediate reagent
PubChem CID: 8471
Canonical SMILES: CCN(CC)CC

Acetonitrile
PubChem CID 6342
Canonical SMILES: CC#N

Tert Butyl 6-Hydroxy-Hexanoate
http://www.trc-canada.com/details.php?CatNumber=B691995
ChemSpider ID: 14090176
CC(C)(C)OC(=O)CCCCCO
CC(C)(C)OC(=O)CCCCCO   JME

Malonyl Dichloride
PubChem CID: 74269
Canonical SMILES: C(C(=O)Cl)C(=O)Cl

ethylenediamine
PubChem CID 3301
Canonical SMILES : C(CN)N

Pyridine
PubChem CID 1049
Canonical SMILES: C1=CC=NC=C1

Diethyl Malonate
PubChem CID 7761
Canonical SMILES: CCOC(=O)CC(=O)OCC

MES
2-morpholinoethanesulfonic acid
buffer
PubChem CID 78165
Canonical SMILES : C1COCCN1CCS(=O)(=O)O

copper(2+) dichloride
radioisotope
PubChem CID 169664
Canonical SMILES : [Cl-].[Cl-].[Cu+2]

DL-Lactide

3,6-Dimethyl-1,4-dioxane-2,5-dione
PubChem CID 7272
Canonical SMILES : CC1C(=O)OC(C(=O)O1)C

stannous octate
Tin(II) 2-ethylhexanoate
PubChem CID 9318
Canonical SMILES : CCCCC(CC)C(=O)[O-].CCCCC(CC)C(=O)[O-].[Sn+2]

Di-Tert-Butyl 4-Amino-4-[2-(Tert-Butoxycarbonyl)Ethyl] Heptanedioate
Newkome dendrimer first generation
Newkome GR et al J. Org. Chem. 56:7162-7167 (1991)
http://www.frontiersci.com/detail.php?FSIcat=NTN1963
CC(C)(C)CC(=O)CCC(N)(CCC(=O)CC(C)(C)C)CCC(=O)CC(C)(C)C JME

1-HOBT
1-Hydroxy Benzotriazole
PubChem CID 75771
Canonical SMILES: C1=CC=C2C(=C1)N=NN2O

DCC
Dicyclohexyl Carbodiimide
PubChem CID: 10868
Canonical SMILES: C1CCC(CC1)N=C=NC2CCCCC2

EtOH
ethanol
PubChem CID: 702
Canonical SMILES: CCO

Ammonium Formate
formic acid
PubChem CID 2723923
Canonical SMILES: C(=O)[O-].[NH4+]

Pyropheophorbide a
3(1),3(2)-Didehydrophytochlorin
Photosensitizer
PubChem CID: 5489042
Canonical SMILES:
CCC1=C2C=C3C(=C4C(=O)CC(=C5C(C(C(=N5)C=C6C(=C(C(=CC(=C1C)N2)N6)C=C)C)C
)CCC(=O)O)C4=N3)C

Tert-Butyl-Aminobutylcarbamate
Tert-Butyl N-(4-Aminobutyl)Carbamate
PubChem CID 4351
Canonical SMILES: CC(C)(C)OC(=O)NCCCCN

Fullerene
 C60
PubChem CID 123591
Canonical SMILES: C12=C3C4=C5C6=C1C7=C8C9=C1C%10=C
%11C(=C29)C3=C2C3=C4C4=C5C5=C9C6=C7C6=C7C8=C1C1=C8C%10=C%10C
%11=C2C2=C3C3=C4C4=C5C5=C%11C%12=C(C6=C95)C7=C1C1=C%12C5=C
%11C4=C3C3=C5C(=C81)C%10=C23

Hydrogen Tetrachloroaurate
PubChem CID: 28133
Canonical SMILES: [H+].Cl[Au-](Cl)(Cl)Cl

DBU
1,8-Diazabicyclo[5.4.0]undec-7-ene
Catalyst
PubChem CID 81184
Canonical SMILES: C1CCC2=NCCCN2CC1

DMA
9,10-Dimethylanthracene
PubChem CID 13076
Canonical SMILES: CC1=C2C=CC=CC2=C(C3=CC=CC=C13)C

Carbon Tetrabromide
PubChem CID 11205
Canonical SMILES: C(Br)(Br)(Br)Br

Sodium Chloroaurate
PubChem CID 27127
Canonical SMILES: [Na+].Cl[Au-](Cl)(Cl)Cl

Hydrogen Tetrachloroaurate
PubChem CID: 28133
Canonical SMILES: [H+].Cl[Au-](Cl)(Cl)Cl

CTAB
Hexadecyltrimethylammonium Bromide
Cationic surfactant
PubChem CID 5974
Canonical SMILES: CCCCCCCCCCCCCCCC[N+](C)(C)C.[Br-]

Silver Nitrate
Surface specific surfactant
Component of growth solution
PubChem CID 24470
Canonical SMILES: [N+](=O)([O-])[O-].[Ag+]

Acetone
Solvent and antiseptic agent
PubChem CID 180

Canonical SMILES: CC(=O)C

Cyclohexane
Nonpolar solvent
PubChem CID 8078
Canonical SMILES: C1CCCCC1

tert-Butyl 2-Aminoethylcarbamate
Description N-Boc-ethylenediamine
Converts completely carboxylic acids to amides?
PubChem CID 187201
Canonical SMILES: CC(C)(C)OC(=O)NCCN

Epicatechin Gallate
PubChem CID 65056
Canonical SMILES:
C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)OC(=O)C4=CC(=C(C(=C4)O)O)O

Catechin
PubChem CID 9064
Canonical SMILES: C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O

Catechin Gallate
PubChem CID 65064
Canonical SMILES: Canonical SMILES:
C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)
O)O

Epicatechin
PubChem CID 72276
Canonical SMILES: C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O

Epigallocatechin
PubChem CID 65084
Canonical SMILES: C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)O

Epigallocatechin Gallate
PubChem CID 65064
Canonical SMILES:
C1C(C(OC2=CC(=CC(=C21)O)O)C3=CC(=C(C(=C3)O)O)O)OC(=O)C4=CC(=C(C(=C4)O)
O)O

HBTU
N,N,N',N'-Tetramethyl-O-(1H-Benzotriazol-1-yl)Uronium
Hexafluorophosphate
PubChem CID 2733084
Canonical SMILES: CN(C)C(=[N+](C)C)ON1C2=CC=CC=C2N=N1.F[P-](F)(F)(F)
(F)F

NHS
N-hydroxysuccinimide
chemical modification reagent
PubChem CID 80170
Canonical SMILES : C1CC(=O)N(C1=O)O

sulfo-NHS
N-hydroxysulfosuccinimide
chemical modification reagent
PubChem CID: 133909
Canonical SMILES C1C(C(=O)N(C1=O)O)S(=O)(=O)O

taurocholic acid
ubChem CID 23666345
Canonical SMILES : CC(CCC(=O)NCCS(=O)(=O)
[O-])C1CCC2C1(C(CC3C2C(CC4C3(CCC(C4)O)C)O)O)C.[Na+]

Silver Nitrate
Surface specific surfactant ?
PubChem CID 24470
Canonical SMILES: [N+](=O)([O-])[O-].[Ag+]

AS
Ascorbic Acid
Oxidation inhibitor
PubChem CID 6981
Canonical SMILES: C(C(C1C(=O)C(=C(O1)O)O)O)O

AminoSPARK®680/VivoTag 680
Description Amine-reactive near-infra-red fluorochrome
http://www.visenmedical.com/products/fluorescence_agents/labeling_agents/technical_support/index.html

pDsRed1-N1 DNA

Red fluorescent vector expressing a fusion of human RanGAP1 - GTPase activator for the nuclear Ras-related regulatory protein Ran, converting it to the putatively inactive GDP-bound state and the red fluorescent protein.

Carboxymethyl-dextran CAS Number 9044-05-7

FA
Folic acid
N-[p-[[(2-amino-4-hydroxy-6-pteridinyl) methyl]-amino]benzoyl]-L-glutamic acid,
B complex vitamin
PubMed CID: 6037

Canonical SMILES:
C1=CC(=CC=C1C(=O)NC(CCC(=O)O)C(=O)O)NCC2=CN=C3C(=N2)C(=O)N=C(N3)N
Inherent Function targeting
Description Targeting folate receptor
Glycosylphosphatidylinositol (GPI)-linked membrane glycoprotein
overexpressed
in variety of tumors

Gemcitabine
Chemotherapeutic drug
PubChem CID 60750
Canonical SMILES : C1=CN(C(=O)N=C1N)C2C(C(C(O2)CO)O)(F)F
function therapy
It replaces one of the building blocks of nucleic acids, in this case
cytidine, during DNA replication.
The process arrests tumor growth, as only one additional nucleoside
can be attached to the "faulty"
nucleoside, resulting in apoptosis.

MTX
Methotrexate - Chemotherapeutic drug
PubChem CID: 126941
Canonical SMILES:
CN(CC1=CN=C2C(=N1)C(=NC(=N2)N)N)C3=CC=C(C=C3)C(=O)NC(CCC(=O)O)C(=O)O
Inherent Function therapeutic
Description Inhibits dihydrofolic acid reductase. Interferes with DNA
synthesis,
repair, and cellular replication of cells in malignant tissues which
proliferation
is greater than in most normal tissues.

coat PL-PEG2000-NH2
DSPE-PEG2000-Amine
          (1,2-distearoyl-sn-glycero-3-phosphoethanolamine-N-(amino
(polyethyleneglycol)2000
          http://www.avantilipids.com/ProductInfo.asp?prodnum=880128

DSPE
1,2-distearoyl-sn-glycero-3-phosphoethanolamine
PubChem CID 447078
Canonical SMILES: CCCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)
(O)OCCN)OC(=O)CCCCCCCCCCCCCCCCC
zwitterionic phospholipid with double C18 acyl chains

NHS-PEG-BOC-3400
Description Tert-Butyloxycarbonyl-PEG-N-Hydroxysuccinimide
http://www.nektar.com

Diphenyl Phosphoryl Chloride
A component of SDPP - N-hydroxysuccinimido diphenyl phosphate

Luo Y, Bernshaw NJ, Lu ZR, Kopecek J, Prestwich GD
Targeted delivery of doxorubicin by HPMA copolymer-hyaluronan bioconjugates
Pharm Res 19:396-402 (2002) PMID: 12033370
PubChem CID: 75654
 Canonical SMILES: C1=CC=C(C=C1)OP(=O)(OC2=CC=CC=C2)Cl

doxorubicin
chemotheraputic agent
PubChem CID: 31703
Canonical SMILES
CC1C(C(CC(O1)OC2CC(CC3=C(C4=C(C(=C23)O)C(=O)C5=C(C4=O)C=CC=C5OC)O)(C(=O)CO)O)N)O
intercalates with DNA inducing single and double-strand breaks in DNA interfering
with DNA replication and RNA synthesis

NHS
N-Hydroxysuccinimide
A component of SDPP - N-hydroxysuccinimido diphenyl phosphate
Luo Y, Bernshaw NJ, Lu ZR, Kopecek J, Prestwich GD
Targeted delivery of doxorubicin by HPMA copolymer-hyaluronan bioconjugates
Pharm Res 19:396-402 (2002) PMID: 12033370
PubChem CID: 80170
Canonical SMILES: C1CC(=O)N(C1=O)O

 5'-NH2 A10 PSMA Aptamer
5'-NH2 modified A10 Prostate Specific Membrane Antibody Aptamer
 Aptamer binds to the prostate-specific membrane antigen (PSMA) on the surface of
 prostate cancer (PCa) cells.
Target antigen PSMA: Cell surface glycoprotein expressed predominantly in prostate secretory
acinar epithelium and prostate cancer cells as well as in several extraprostatic tissues,
species: human

Glycidol
demulsifier
PubChem CID: 11164
Canonical SMILES: C1C(O1)CO

Amphiphilic polymer - 40% octylamine-modified
                polyacrylic acid,2000 units/QD
                Wu et al http://dx.doi.org/10.1038/nbt764

5-Carboxyfluorescein N-succinimidyl ester
    MW: 473.387900 g/mol | MF: C25H15NO9 PubChem 1:   CID: 4564399
 Canonical SMILES:

C1CC(=O)N(C1=O)OC(=O)C2=CC(=C(C=C2)C3=C4C=CC(=O)C=C4OC5=C3C=CC(=C5)O)C(=O)O

Carboxyfluorescein
Fluorescent dye
5(6)-Carboxyfluorescein
MW 376.32 MF C21H12O7
lambda_ex 492 nm lambda_em 517 nm
http://www.sigmaaldrich.com/catalog/search/ProductDetail/FLUKA/21877}
PubChem CID 123755
Canonical SMILES:
C1=CC2=C(C=C1C(=O)O)C(=O)OC23C4=C(C=C(C=C4)O)OC5=C3C=CC(=C5)O

FITC - Fluorescein Isothiocyanate - fluorescent probe
MW: 389.380740 g/mol | MF: C21H11NO5S PubChem CID: 18730
Canonical SMILES:
C1=CC2=C(C=C1N=C=S)C(=O)OC23C4=C(C=C(C=C4)O)OC5=C3C=CC(=C5)O

Alexa Fluor 488 carboxylic succinimidyl ester
http://products.invitrogen.com/ivgn/en/US/adirect/invitrogen?cmd=catProductDetail&entryPoint=adirect&productID=A20000&CID=AFLBC&messageType=catProductDetail

Phosphatidylethanolamine (NBD)
Fluorophore conjugated to the head group of phosphatidylethanolamine
http://www.avantilipids.com/FluorescentHeadgroupPhosphatidylethanolamine.asp

Phosphatidylethanolamine (Lissamine Rhodamine B)
Fluorophore conjugated to the head group of phosphatidylethanolamine
http://www.avantilipids.com/FluorescentPELissamineRhodamine.asp

1,2-Dioleoyl-sn-Glycero-3-Phosphoethanolamine-N-(Carboxyfluorescein)
Fluorophore conjugated to the head group of phosphatidylethanolamine
http://www.avantilipids.com/ProductStructures.asp?n=810332

ODA
octadecylamine
PubChem CID 15793
Canonical SMILES : CCCCCCCCCCCCCCCCCCN

Fluorescein
Fluorophore
PubChem CID 16850
Canonical SMILES:
C1=CC=C2C(=C1)C(=O)OC23C4=C(C=C(C=C4)O)OC5=C3C=CC(=C5)O

BODIPY Fluorophore
PubChem CID 25058173
Canonical SMILES: [B-]1(N2C=CC=C2C=C3[N+]1=CC=C3)(F)F

Carbon Tetrabromide
PubChem CID 11205
Canonical SMILES: C(Br)(Br)(Br)Br

DIPEA
N,N-Diisopropylethylamine
PubChem CID 81531
Canonical SMILES: CCN(C(C)C)C(C)

t-Boc-glycine
PubChem 78288
Canonical SMILES: CC(C)(C)OC(=O)NCC(=O)O

PBA
phenylboronic acid
PubChem CID 66827
Canonical SMILES : B(C1=CC=CC=C1)(O)O

DIC
N,N'-Diisopropylcarbodiimide
PubChem CID 12734
Canonical SMILES : CC(C)N=C=NC(C)C

coat SDS
Sodium dodecyl sulfate; surfactant
MW: 288.379270 g/mol | MF: C12H25NaO4S PubChem CID: 3423265
Canonical SMILES: CCCCCCCCCCCCOS(=O)(=O)[O-].[Na+]

Sodium Carbonate
PubChem CID 10340
Canonical SMILES: C(=O)([O-])[O-].[Na+].[Na+]

Sodium Hydrogen Carbonate
PubChem CID 516892
Canonical SMILES: C(=O)(O)[O-].[Na+]

modification 3H
Tritium
MW: 3.016049 g/mol | MF: H PubChem CID: 5460633
Canonical SMILES: [H]
Isomeric SMILES: [3H]

Boc-Asp(OBzl)-OSu
Boc-L-aspartic acid 4-benzyl 1-(hydroxysuccinimide) ester
PubChem CID 13517798
Canonical SMILES : CC(C)
(C)OC(=O)NC(CC(=O)OCC1=CC=CC=C1)C(=O)ON2C(=O)CCC2=O

modification c(RGDfC) cyclo-(Arg-Gly-Asp-D-Phe-Lys)
cyclic peptide
Alpha-nu-beta-3 integrin targeting agent
Inherent function
targeting
Targeting alpha-nu-beta-3 integrins - cell adhesion receptors involved in cell-extracellular matrix and cell-cell interactions

PGA
Poly-l-glutamic acid (PGA) sodium salt (Mw = 15,000~50,000)
Sigma-Aldrich P4761

Polyglutamic Acid
PubChem CID: 33032
Canonical SMILES: C(CC(=O)O)C(C(=O)O)N

PLL
Poly(L-lysine) hydrobromide (Mw =15 000–30 000 g mol)
Sigma-Aldrich P7890

Poly-L-lysine hydrobromide
PubChem SID: 24898886
Canonical SMILES: C(CCN)CC(C(=O)O)N.Cl

silica
silicon dioxide
PubChem CID 24261
Canonical SMILES : O=[Si]=O

Tat
Cell penetrating peptide and trans-activating transcriptional activator
from Human Immunodeficiency Virus 1

TEOS
Tetraethyl Orthosilicate
PubChem CID 6517
Canonical SMILES: CCO[Si](OCC)(OCC)OCC

MPS
3-(Methacryloxy) Propyl Triethoxysilane
PubChem CID 17318
Canonical SMILES: CC(=C)C(=O)OCCC[Si](OC)(OC)OC

MPTS
(3-Mercaptopropyl)trimethoxysilane
PubChem CID 20473
Canonical SMILES : CO[Si](CCCS)(OC)OC

NIPAM
N-isopropylacrylamide
PubChem CID 16637
Canonical SMILES: CC(C)NC(=O)C=C

Linoleic Acid
Component of pine-nut oil
PubChem CID 3931
Canonical SMILES: CCCCCC=CCC=CCCCCCCCC(=O)O

Pinolenic Acid
Component of pine-nut oil
PubChem CID 5312493
Canonical SMILES: CCCCCC=CCC=CCCC=CCCCC(=O)O

Citric Acid
PubChem CID 311
Canonical SMILES: C(C(=O)O)C(CC(=O)O)(C(=O)O)O

Ammonia
colorless alkaline gas
PubChem CID 222
Canonical SMILES: N

Cadmium Perchlorate
PubChem CID 203082
Canonical SMILES: [O-]Cl(=O)(=O)=O.[O-]Cl(=O)(=O)=O.[Cd+2]

DSPC
1,2-distearoyl-glycero-3-phosphocholine
PubChem CID 94190
Canonical SMILES : CCCCCCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)OC(=O)CCCCCCCCCCCCCCCCC

MHPC
1-myristoyl-2-hydroxy-sn-glycero-3-phosphocholine
zwitterionic phospholipid with a single C14 acyl chain
PubChem CID 460604
Canonical SMILES : CCCCCCCCCCCCCC(=O)OCC(COP(=O)([O-])OCC[N+](C)(C)C)O

(TMS)2S
bis(trimethylsilyl) sulfide
PubChem CID 76920
Canonical SMILES : C[Si](C)(C)S[Si](C)(C)C

ethylene glycol
PubChem CID 174
Canonical SMILES : C(CO)O

HETM
hexamethylene tetramine
PubChem CID 4101
Canonical SMILES : C1N2CN3CN1CN(C2)C3

potassium nitrate
PubChem CID 24434
Canonical SMILES : [N+](=O)([O-])[O-].[K+]

dichlorotin
PubChem CID 24479
Canonical SMILES : Cl[Sn]Cl

DSPE-PEG2k
1,2-distearoyl-sn-glycero-3-phosphoethanolamine-N-[methoxy
(polyethylene glycol)-2000] (Avanti Polar Lipids 880120)

DSPE-PEG Amine
1,2-distearoyl-sn-glycero-3-phosphoethanolamine-N-[amino(polyethylene
glycol)-2000]
Avanti Polar Lipids 880128

2'-FU   2'-deoxy-2'-fluorouridine monophosphate
2'-FC   2'-deoxy-2'-fluorocytidine monophosphate http://
www.glenresearch.com/GlenReports/GR17-15.html

trans-1,2-bis(4-pyridyl)-ethylene
1,2-Di-4-pyridylethene
PubChem CID 776222
C1=CN=CC=C1C=CC2=CC=NC=C2

MMA
methyl methacrylate
PubChem CID 6658
Canonical SMILES : CC(=C)C(=O)OC

potassium persulfate
PubChem CID 24412
Canonical SMILES : [O-]S(=O)(=O)OOS(=O)(=O)[O-].[K+].[K+]

MMA-DOTA
1,4,7,10-tetraazacyclododecane-1,4,7-tris-acetic acid-10-
maleimidoethylacetamide (Macrocyclics)

gadolinium chloride hexahydrate
PubChem CID 16211472
Canonical SMILES : O.Cl[Gd](Cl)Cl