

POLYMER- AND SOLID-SUPPORT-NAMES; MKEYWORDS

1. Polymer Names

The datafield POLYMER_NAME can contain up to four entries. Usually, these entries have the following contents:

POLYMER_NAME(1): Description of the polymer backbone
POLYMER_NAME(2): Polymer Backbone Specifier
POLYMER_NAME(3): Name of the Polymer Support
POLYMER_NAME(4): Additional Name

The **description of the polymer backbone** provides a brief characterization of the polymeric framework, using terms such as "2% crosslinked polystyrene", "TentaGel S", or "polyethylene glycol monomethyl ether" (cf. Appendix 1 for a list of examples), based on the data given in the publication. If not specified otherwise, the term "crosslinked" always refers to the standard type of crosslinker for that particular resin, e. g. to divinylbenzene-crosslinked polystyrene in the expression "crosslinked polystyrene".

The **polymer backbone specifier** was devised to facilitate searching for particular polymer types via abbreviated terms such as "PS" (giving all reactions on standard polystyrene supports — including "polymer derivatization" reactions, which cannot be found by searches using the MOLEXTREG), "soluble PS" (leading to all reactions on non-crosslinked polystyrene) or "PS-PEG" (for all reactions on TentaGel, ArgoGel, or other PEG-grafted polystyrene polymers) etc. A complete list of all specifiers used in SPORE is given in Appendix 2.

While the first two entries describe the polymer framework, the **name of the polymer support** relates to the complete structure of the polymeric support (i. e., the polymer part of the support without the linker, or the complete support if no linker is present). The name cited here will be one of the names (SYMBOLs; without the "Generic:" term) assigned to the corresponding generic structure of the polymer support, which is connected to the reaction via its MOLEXTREG.

In some cases, an **additional name** can be present as well. Thus, the term "Merrifield resin" (an expression with a context-dependent meaning in the literature) is assigned to reactions in which the ligand is attached to standard 1-2% crosslinked

amino-, thio-, or oxymethylpolystyrene beads (without any additional linker or spacer).

If expressions in the different categories are identical (e.g. "cellulose" as backbone specifier and polymer support name), one entry is omitted and the reaction will have only two entries in the POLYMER_NAME datafield.

2. Solid Support Name(s)

The field SOLID_SUPPORT_NAME will usually have only one entry; a second entry may exist, however, in some cases (e. g. the entry "Merrifield resin" for the reactions described above).

The particular name assigned is based on the data given in the publication. It must, however, be identical to one of the SYMBOLs of the corresponding generic solid support molecule (without the "Generic:" term) having the MOLEXTREG cited in the SOLID_SUPPORT:MOLEXTREG datafield.

3. The Datafield MKEYWORDS

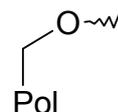
The datafields POLYMER_NAME and SOLID_SUPPORT_NAME are based on reactions; on the molecular level, some entries in the field MKEYWORDS facilitate searching for particular structural types of polymers (cf. Appendix 3 for a list of these terms).

Several terms are identical to those used for the polymer backbone specifier, even though the meaning may be more general in some cases. Thus, the MKEYWORD "PS" relates to all types of non-crosslinked or crosslinked polystyrene, independent of the crosslinker present in the polymer of a particular reaction (a distinction between crosslinkers is not possible here since all these polymers have the same structural representation [zero- or monovalent "Pol"], and polystyrene derivatives with different polymeric frameworks are thus represented by the same molecule in the database).

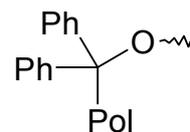
4. Examples: Assignment of Polymer and Solid Support Names

4.1 Supports without a linker

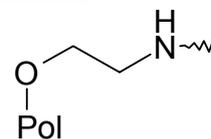
<i>MOLEXTREG:</i>	PSOX
<i>Polymer Names:</i>	1% crosslinked polystyrene PS oxymethylpolystyrene Merrifield resin
<i>Solid Support Name(s):</i>	oxymethylpolystyrene Merrifield resin



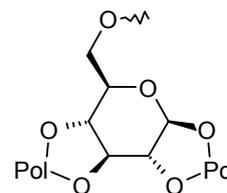
MOLEXTREG: PTRX
 Polymer Names: 2% crosslinked polystyrene
 PS
 trityl resin
 Solid Support Name(s): trityl resin



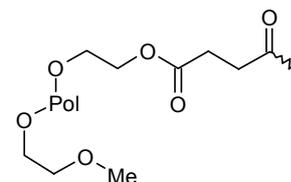
MOLEXTREG: TSNX
 Polymer Names: TentaGel S
 PS-PEG
 TentaGel S-NH2
 Solid Support Name(s): TentaGel S-NH2



MOLEXTREG: CSOX
 Polymer Names: paper
 cellulose
 (No 3rd entry; Name(3) = Name(1-2))
 Solid Support Name(s): paper

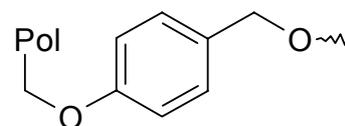


MOLEXTREG: EMOS [succinyl = spacer, not linker]
 Polymer Names: polyethylene glycol monomethyl ether
 MPEG
 succinyl-MeO-PEG
 Solid Support Name(s): succinyl-MeO-PEG

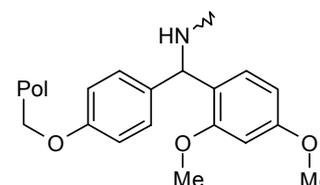


4.2 Supports with a linker

MOLEXTREG: PSOX1200
 Polymer Names: crosslinked polystyrene
 PS
 oxymethylpolystyrene
 Solid Support Name(s): Wang resin



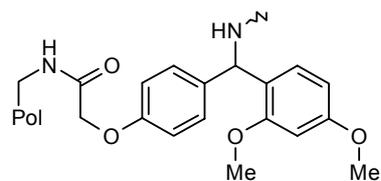
MOLEXTREG: PSOX2400
 Polymer Names: crosslinked polystyrene
 PS
 oxymethylpolystyrene
 Solid Support Name(s): Rink amide resin



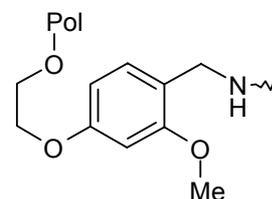
MOLEXTREG: PSNA2400
 Polymer Names: crosslinked polystyrene
 PS

oxyacetyl-
 aminomethyl-PS
 Solid Support Name(s):

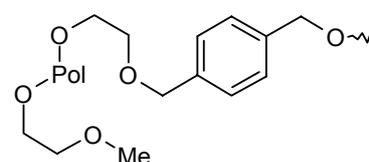
Rink amide AM resin



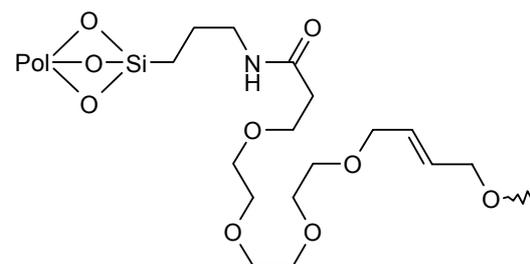
MOLEXTREG: TSOX1310
 Polymer Names: ArgoGel
 PS-PEG
 PS-PEG-OH
 Solid Support Name(s): ArgoGel-MB-NH2 resin



MOLEXTREG: EMOX1206
 Polymer Names: polyethylene glycol monomethyl ether
 MPEG
 (No 3rd entry; Name(3) = Name(1-2))
 Solid Support Name(s): MPEG-DOX

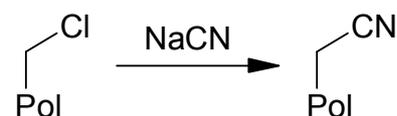


MOLEXTREG: GPAX0003
 Polymer Names: controlled pore glass
 glass
 aminopropyl-CPG
 Solid Support Name(s): HYCRON-aminopropyl-CPG



4.3 Polymer derivatizations in the absence of a linker and ligand

MOLEXTREG: (No entry)
 Polymer Names: 2% crosslinked polystyrene
 PS
 Solid Support Name(s): (No entry)



Appendix 1: Examples for POLYMER_NAME(1) Entries

MOLEXTREG	POLYMER_NAME(1)
A...	poly(dimethylacrylamide) poly(dimethylacrylamide) (PepSyn gel resin) poly(acrylamide/N-isopropylacrylamide) Expansin Macrosorb SPR 250 polyamide-Kieselguhr polyacrylic acid polyacrylic acid grafted polypropylene membranes poly(2-oxyethyl methacrylate-co-ethylene dimethacrylate) EDMA-crosslinked polymethacrylate PE pins radiation-grafted with methacrylic acid/dimethylacrylamide poly(MA/DMA)-grafted polyethylene pins SynPhase-MD O-series crowns (MA/DMA) MA/DMA crowns MA/DMA-grafted SynPhase lanterns (D-series)
BM..	2% EDMA-crosslinked poly(PEG methacrylate)
BP..	PEGA resin PEGA-800 PEGA-1900 PEGA 1900/130 macrobeads magnetite-containing PEGA resin
C...	paper cellulose cellulose powder cellulose membranes Perloza MT-100 cotton cotton disks sucrose layer on a microchip
D...	Sepharose 6B Affi-Gel 10 agarose layer on a microchip polygalactoside layer on a microchip
EB..	hyperbranched pentaerythritol/dimethylpropionic acid copolymer
EC..	(polyethylene glycol)6-cyclotriphospazene
EE..	core-ethylated dendritic polyglycerol
EG..	dendritic polyglycerol
EM..	polyethylene glycol monomethyl ether
EN../ED..	polyethylene glycol ("ED.." for dendritic derivatives)
EP..	Sunbright PTE-2000 tetra(polyethylene glycol)-pentaerythritol

MOLEXTREG	POLYMER_NAME(1)
F...	carbon felt (Actitex 1500-1) single-wall carbon nanotubes activated carbon glassy carbon disc
G...	glass plates microscope slides glass-encased microchips controlled pore glass (CPG) controlled pore glass (LCAA-CPG) controlled pore glass (LCAMA-CPG) borosilicate glass silica gel silica gel 60 silica gel (Merck 60) MCM-41 silica siliceous MCM-41 mesoporous silica mesoporous molecular sieves silica ceramic particles Aerosil A-200 Fractosil xerogel silica xerogel organically modified xerogel (OMX-NH ₂) permeable CPG layer on an electrode array
I...	polypyrrole polypyrrole film on graphite felt electrodes
J...	polythiophene
K...	Sephadex G-15
L...	crosslinked ethoxylate acrylate resin
M...	p-xylylene-crosslinked polyethylene imine 2% Tren-crosslinked poly(p-xylylene/ethylene imine)
N...	Nafion NR50
O...	POEPOP resin POEPOP-400 POEPOP-1000 POEPOP-1500
P... (Merrifield-type)	crosslinked polystyrene 1% crosslinked polystyrene 2% crosslinked polystyrene 1.5% crosslinked polystyrene 1 or 2% crosslinked polystyrene

MOLEXTREG	POLYMER_NAME(1)
P... (highly crosslinked and/or high capacity)	highly crosslinked polystyrene 5-7% crosslinked polystyrene 20% crosslinked polystyrene 50% crosslinked polystyrene crosslinked polystyrene (Amberlite XE-305) 6% crosslinked polystyrene (Amberlite XE-298A) 20% crosslinked polystyrene (polyHIPE) highly crosslinked polystyrene (Argo-X203) highly crosslinked polystyrene (ArgoPore) high-capacity crosslinked polystyrene macrobeads
P... (non-crosslinked)	non-crosslinked polystyrene
P... (on carrier)	polystyrene-grafted crowns SynPhase PS macro crowns SynPhase PS lanterns SynPhase PS lanterns (D-series) polystyrene-grafted polypropylene MicroTubes polystyrene-grafted PTFE MicroTubes polystyrene-grafted poly(tetrafluoroethylene) polystyrene colloid on aminated polyethylene (Porex X-4920) crosslinked polystyrene beads in polyethylene plugs magnetic polystyrene-coated composite paramagnetic crosslinked polystyrene support
P... (other crosslinkers than DVB)	JandaJel 2% crosslinked JandaJel 5% (PTHF)9.5-crosslinked polystyrene 2% 1,4-butanediol dimethacrylate-crosslinked polystyrene 2% 1,6-hexanediol diacrylate-crosslinked polystyrene 50% PEG1000 diacrylate-crosslinked polystyrene 50% PEG1000 di(4-vinylbenzyl ether)-crosslinked polystyrene 4% TTEGDA-crosslinked polystyrene 3 wt.% diethylene glycol dimethacrylate-crosslinked polystyrene 2.7 wt.% triethylene glycol dimethacrylate-crosslinked polystyrene
P... (modified polystyrene resins)	poly(trifluorostyrene) 20% DVB-crosslinked styrene/ethylstyrene/2,5-diphenyl-4-vinyloxazole copolymer 5% (tetraethylene glycol)-OME on 2% crosslinked polystyrene 2% DVB-crosslinked styrene/7% MEEVB copolymer divinylbenzene/ethylstyrene copolymer (polyHIPE) fluorine-labeled crosslinked polystyrene polystyrene chains on 1% crosslinked polystyrene polynorbornene-ROMP on crosslinked polystyrene Jeffamine ED-600/triazine on 1% crosslinked polystyrene dendritic polystyrene-graft-polyglycerol hybrid polymer NovaGel Champion I resin

MOLEXTREG	POLYMER_NAME(1)
R...	<p>polynorbornene-ROMP soluble polynorbornene-ROMP poly(norbornene-co-norbornenedimethanol)-ROMP hexahydrodimethanonaphthalene-crosslinked polynorbornene-ROMP polyoxanorbornene-ROMP 4-dinorbornenylbenzene-crosslinked polyoxanorbornene-ROMP norbornadiene-crosslinked polyoxanorbornene-ROMP 1% bis(norbornenylmethyl) ether-crosslinked polynorbornene-ROMP perhydro 1% bis(norbornenylmethyl) ether-crosslinked polynorbornene-ROMP</p>
S...	<p>SPOCC resin <i>(not yet used)</i> SPOCC-400 SPOCC-1500</p>
T...	<p>PEG-grafted polystyrene PEG-grafted 1% crosslinked polystyrene polyethylene glycol-polystyrene graft copolymer polyethylene glycol-grafted polystyrene highly loaded PEG-coated polystyrene (HLP) microporous PEG-PS graft PEG-PS resin TentaGel TentaGel S TentaGel M TentaGel HL TentaGel macrobeads NovaSyn TG resin ArgoGel dipropyl-PEG-1500-crosslinked PS-PEG (POEPS-3) paramagnetic Jeffamine XTJ-502-grafted polystyrene magnetite-containing Jeffamine(PEG900)-grafted polystyrene</p>
U...	<p>ChemMatrix resin NovaPEG resin</p>
VA..	poly(styrene-co-allyl alcohol)
VE..	PEG-grafted crosslinked polyvinyl alcohol
VL..	2% BDDVE-crosslinked BDVE/MeBDVE copolymer (<i>BDVE = 1,4-butanediol vinyl ether</i>)
VP..	crosslinked poly(4-vinylpyridine)
VS..	<p>Merckogel OR 1000000 epichlorohydrin-crosslinked polyvinyl alcohol acrylate/polyvinyl alcohol copolymer on an electrode array</p>
W...	polyisobutylene (Glissopal 1000 or 2300)

**Appendix 2: Complete List of Polymer Backbone Specifiers
(usually POLYMER_NAME(2))**

MOLEXTREG	Specifier	Used for polymer backbones of:
A...	PA	All polyacrylamide-type resins, including PA grafted on other carriers (as in pins or crowns)
	polyacrylate	Resins based on polyacrylic acid and ester derivatives
BM..	PEG-MA	EDMA-crosslinked poly(PEG methacrylate)
BP..	PEGA	PEGA resin; PEG-crosslinked polyacrylamide with PEG side chains
C...	cellulose sucrose-based polymer	Cellulose, paper, Perloza resin, cotton For sucrose-based coatings on microchips
D...	agarose	Agarose, Sepharose, Affi-Gel
EB..	Boltorn polyester	Boltorn H-40, Boltorn H-50
EC..	PEG6-cycloP3N3	Hexa(PEG)-substituted cyclotriphosphazene, PEG stealth star
EE..	Et-PG	Core-ethylated dendritic polyglycerol
EG..	PG	Dendritic polyglycerol
EM..	MPEG	Polyethylene glycol monomethyl ether, MeO-PEG, MPEG
EN..	PEG	Polyethylene glycol (bifunctional), PEG
EP..	PEG4-pentaerythritol	PTE-2000; four PEG chains attached to a pentaerythritol core, star-PEG
F...	carbon	activated carbon, carbon felt, glassy carbon, carbon nanotubes
G...	glass	Glass, borosilicate glass, controlled pore glass, CPG, LCAA-CPG
	silica	Silica gel, silica ceramic particles, molecular sieves, MCM-41, Fractosil, Aerosil A-200
I...	(1) polypyrrole (2) electropolymer	Polypyrrole films obtained by electropolymerization
J...	(1) polythiophene (2) electropolymer	Polythiophene films generated by anodic polymerization

MOLEX TREG	Specifier	Used for polymer backbones of:
K...	Dextran	Dextran, Sephadex
L...	CLEAR	Co-polymers of the branched crosslinker trimethylolpropane ethoxylate (14/3 EO/OH) triacrylate
M...	PEI	polyethylene imine
N...	Nafion	Nafion fluoropolymers
O...	POEPOP	POEPOP resin; PEG-crosslinked polyoxypropylene with PEG side chains
P...	PS	Divinylbenzene-crosslinked polystyrene, polystyrene grafted on other carriers (as in pins, crowns)
	soluble PS	Non-crosslinked, soluble polystyrene
	PTHF-PS	Polystyrene with a THF- or poly(THF)-derived crosslinker; "JandaJel"
	DEGDMA-PS	Polystyrene crosslinked with diethylene glycol dimethacrylate
	TEGDMA-PS	Polystyrene crosslinked with triethylene glycol dimethacrylate
	TTEGDA-PS	Polystyrene crosslinked with tetraethylene glycol diacrylate
	HDODA-PS	Polystyrene crosslinked with 1,6-hexanediol diacrylate
	BDODMA-PS	Polystyrene crosslinked with 1,4-butanediol dimethacrylate
	MEEVB-PS	Styrene/DVB/p-(methoxyethoxyethoxy)vinylbenzene copolymer
	(PEG diacrylate)-PS	Polystyrene crosslinked with diacrylates of PEG (400, 1000 etc.)
	(PEG-DVBE)-PS	Polystyrene crosslinked with PEG di(4-vinylbenzyl ether)
	(MPEG-CO-NH-CH ₂)-PS	NovaGel; Champion I; crosslinked aminomethyl-PS, partly substituted with carbamate-anchored MeO-PEG chains
	diphenyloxazolyl-PS	Copolymer of styrene, 2,5-diphenyl-4-vinylazole and ethylstyrene
	PTFS	Poly(trifluorostyrene)
	PG-PS	Dendritic polyglycerol on crosslinked polystyrene
	Rasta-PS	Polystyrene chains on a crosslinked polystyrene core
ROMP-PS	ROM polymer on crosslinked polystyrene core	

MOLEX TREG	Specifier	Used for polymer backbones of:
R...	ROMP	Crosslinked or non-crosslinked insoluble ROM polymer obtained from norbornene or oxanorbonene derivatives
	soluble ROMP	Non-crosslinked soluble polymer of this type
	H-ROMP	Hydrogenated ROM polymer without olefinic groups
S...	SPOCC	SPOCC resin; PEG-crosslinked polyoxetane with PEG side chains
T...	PS-PEG	PEG-grafted polystyrene, TentaGel, ArgoGel, POEPS-3
U...	CM	ChemMatrix (CM) resin, NovaPEG resin
VA..	polyallyl ester	Esters of poly(styrene-co-allyl alcohol)
VE..	PVA-PEG	PEG-grafted crosslinked polyvinyl alcohol
VL..	SLURPS	Copolymers of 1,4-butanediol vinyl ether derivatives
VP..	PVP	Derivatives of poly(4-vinylpyridine)
VS..	PVA	Derivatives of polyvinyl alcohol, Merckogel, crosslinked polyvinyl alcohol (PVA-OH)
W...	PIB	Polyisobutylene, Glissopal

Appendix 3: List of Selected MKEYWORDS

1. Generic Molecules

<u>Protecting groups:</u>	<i>protecting group, generic structure</i>
<u>Supports without a linker:</u>	<i>polymer support, solid support, generic structure</i>
<u>Supports with a linker:</u>	<i>linker, solid support, generic structure</i>

All generic molecules: Additional keywords describing the linking functionality (e.g., *oxy, dioxy, amino, hydrazino, ammonio, thio, sulfonyl, carbonyl, silyl, etc.*)

2. Polymer Types (MKEYWORDS for all polymer-bound molecules)

MOLEXTREG ^{†)}	MKEYWORDS
A... (amide)	<i>PA, polyacrylamide</i>
A... (ester)	<i>PA, polyacrylate</i>
BM..	<i>PEG-MA, PA-PEG, polyethylene glycol, polyacrylate</i>
BP..	<i>PEGA, PA-PEG, polyethylene glycol, polyacrylamide</i>
C...	<i>cellulose, carbohydrate support</i>
D...	<i>agarose, carbohydrate support</i>
EB..	<i>Boltorn polyester</i>
EC..	<i>PEG6-cycloP3N3, PEG6-stealth star, polyethylene glycol</i>
EE..	<i>Et-PG, polyglycerol</i>
EG..	<i>PG, polyglycerol</i>
EM..	<i>MPEG, PEG, polyethylene glycol</i>
EN..	<i>PEG, polyethylene glycol</i>
EP..	<i>PEG4-pentaerythritol, polyethylene glycol</i>
F...	<i>carbon, electropolymer</i>
G...	<i>glass, silica</i>
I...	<i>polypyrrole, electropolymer</i>
J...	<i>polythiophene, electropolymer</i>

^{†)} Refers to the MOLEXTREG of generic molecules of this structural type

MOLEXTREG ⁺⁾	MKEYWORDS
K...	<i>dextran, carbohydrate support</i>
L...	<i>CLEAR, polyacrylate, polyethylene glycol</i>
M...	<i>PEI, polyethylene imine</i>
N...	<i>Nafion, PTFE</i>
O...	<i>POEPOP, polyoxypropylene, polyethylene glycol</i>
P...	<i>PS, polystyrene</i> (additional mkeywords for special structures: <i>Rasta-PS</i> or <i>ROMP-PS</i> or <i>PG-PS</i> + <i>polyglycerol</i>)
R...	for RC...: <i>ROMP, polynorbornene</i> for RO...: <i>ROMP, polyoxanorbornene</i> for RS...: <i>ROMP, polynorbornene, H-ROMP</i>
S...	<i>SPOCC, polyoxetane, polyethylene glycol</i>
T...	<i>PS-PEG, polystyrene, polyethylene glycol</i>
U...	<i>CM, polyethylene glycol</i>
VA..	<i>polyallyl alcohol, polyallyl ester</i>
VE..	<i>PVA-PEG, polyvinyl alcohol, polyethylene glycol</i>
VL..	<i>polyvinyl alcohol, SLURPS</i>
VP..	<i>polyvinylpyridine, PVP</i>
VS..	<i>polyvinyl alcohol, PVA</i>
W...	<i>PIB, polyisobutylene</i>

⁺⁾ Refers to the MOLEXTREG of generic molecules of this structural type