

SUPPLEMENTARY INFORMATION

UNDERSTANDING POLYMERS THROUGH TRANSFER LEARNING AND EXPLAINABLE AI

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KEYWORDS: AI; White boxing; Transfer learning; Polymer glass transition.

a) Raw acrylates dataset

The dataset used in this work is shown in Table S1.

Table S1

| Name | SMILES | T _g [K] |
|--|---|--------------------|
| Poly[methyl 4-(methacryloyloxy)benzoate] | <chem>C=C(C)C(=O)Oc1ccc(C(=O)OC)cc1</chem> | 379 |
| Poly[methyl 4-(methacrylamido)benzoate] | <chem>C=C(C)C(=O)Nc1ccc(C(=O)OC)cc1</chem> | 453 |
| Poly[methyl 4-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1ccc(C(=O)OC)cc1</chem> | 340 |
| Poly[methyl 3-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1cccc(C(=O)OC)c1</chem> | 311 |
| Poly[methyl 2-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1cccc1C(=O)OC</chem> | 319 |
| Poly[ethyl 4-(methacrylamido)benzoate] | <chem>C=C(C)C(=O)Nc1ccc(C(=O)OCC)cc1</chem> | 441 |
| Poly[ethyl 4-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1ccc(C(=O)OCC)cc1</chem> | 310 |
| Poly[ethyl 2-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1cccc1C(=O)OCC</chem> | 303 |
| Poly[butyl 4-(methacrylamido)benzoate] | <chem>C=C(C)C(=O)Nc1ccc(C(=O)OCCCC)cc1</chem> | 401 |
| Poly[butyl 4-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1ccc(C(=O)OCCCC)cc1</chem> | 286 |
| Poly[4-(cyanomethyl)phenyl methacrylate] | <chem>C=C(C)C(=O)Oc1ccc(CC#N)cc1</chem> | 401 |
| Poly(terbutyl methacrylate) | <chem>C=C(C)C(=O)OC(C)(C)C</chem> | 391 |
| Poly(terbutyl acrylate) | <chem>C=CC(=O)OC(C)(C)C</chem> | 316 |
| Poly(secbutyl methacrylate) | <chem>C=C(C)C(=O)OC(C)CC</chem> | 333 |
| Poly(secbutyl chloroacrylate) | <chem>C=C(Cl)C(=O)OC(C)CC</chem> | 347 |
| Poly(propyl chloroacrylate) | <chem>C=C(Cl)C(=O)OCCC</chem> | 344 |
| Poly(phenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccccc1</chem> | 383 |
| Poly(phenyl acrylate) | <chem>C=CC(=O)Oc1ccccc1</chem> | 323 |
| Poly(pentyl methacrylate) | <chem>C=C(C)C(=O)OCCCCC</chem> | 268 |
| Poly(N-terbutylacrylamide) | <chem>C=CC(=O)NC(C)(C)C</chem> | 401 |
| Poly(n-pentyl acrylate) | <chem>C=CC(=O)OCCCCC</chem> | 216 |
| Poly(N-octylacrylamide) | <chem>C=CC(=O)NCCCCCCCC</chem> | 220 |
| Poly(N-methyl-N-phenylacrylamide) | <chem>C=CC(=O)N(C)c1ccccc1</chem> | 453 |
| Poly(N-isopropylacrylamide) | <chem>C=CC(=O)NC(C)C</chem> | 358 |
| Poly(neopentyl methacrylate) | <chem>C=C(C)C(=O)CC(C)(C)C</chem> | 312 |
| Poly(neopentyl acrylate) | <chem>C=CC(=O)OCC(C)(C)C</chem> | 295 |
| Poly(N-butylacrylamide) | <chem>C=CC(=O)NCCCC</chem> | 319 |
| Poly(N,N-dimethylacrylamide) | <chem>C=CC(=O)N(C)C</chem> | 362 |
| Poly(N,N-diisopropylacrylamide) | <chem>C=CC(=O)N(C(C)C)C(C)C</chem> | 393 |
| Poly(N,N-dibutylacrylamide) | <chem>C=CC(=O)N(CCCC)CCCC</chem> | 333 |
| Poly(N-(1-methylbutyl)acrylamide) | <chem>C=CC(=O)NCC(C)CC</chem> | 380 |
| Poly(methyl fluoromethacrylate) | <chem>C=C(C(F))C(=O)OC</chem> | 357 |
| Poly(methyl fluoroacrylate) | <chem>C=C(F)C(=O)OC</chem> | 404 |
| Poly(methyl chloroacrylate) | <chem>C=C(Cl)C(=O)OC</chem> | 419 |
| Poly(methyl atropate) | <chem>C=C(C(=O)OC)c1ccccc1</chem> | 391 |
| Poly(methyl acrylate) | <chem>C=CC(=O)OC</chem> | 281 |
| Poly(isopropyl methacrylate) | <chem>C=C(C)C(=O)OC(C)C</chem> | 359 |
| Poly(isobutyl methacrylate) | <chem>C=C(C)C(=O)OCC(C)C</chem> | 326 |
| Poly(isobutyl acrylate) | <chem>C=CC(=O)OCC(C)C</chem> | 249 |
| Poly(hexyl methacrylate) | <chem>C=C(C)C(=O)OCCCCC</chem> | 268 |
| Poly(hexyl acrylate) | <chem>C=CC(=O)OCCCCC</chem> | 216 |
| Poly(heptyl acrylate) | <chem>C=CC(=O)OCCCCCCC</chem> | 213 |

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| Poly(heptafluoro-2-propyl acrylate) | <chem>C=CC(=O)OC(F)(C(F)(F)F)C(F)(F)F</chem> | 278 |
| Poly(fluoromethyl acrylate) | <chem>C=CC(=O)OCF</chem> | 288 |
| Poly(ethyl methacrylate) | <chem>C=C(C)C(=O)OCC</chem> | 359 |
| Poly(ethyl fluoromethacrylate) | <chem>C=C(CF)C(=O)OCC</chem> | 316 |
| Poly(ethyl ethacrylate) | <chem>C=C(CC)C(=O)OCC</chem> | 300 |
| Poly(ethyl acrylate) | <chem>C=CC(=O)OCC</chem> | 249 |
| Poly(dodecyl methacrylate) | <chem>C=C(C)C(=O)OCCCCCCCCCCCCC</chem> | 208 |
| Poly(dimethylaminoethyl methacrylate) | <chem>C=C(C)C(=O)OCCN(C)C</chem> | 292 |
| Poly(cyanomethyl acrylate) | <chem>C=CC(=O)OCC#N</chem> | 433 |
| Poly(butyl methacrylate) | <chem>C=C(C)C(=O)OCCCC</chem> | 293 |
| Poly(butyl cyanoacrylate) | <chem>C=C(C#N)C(=O)OCCCC</chem> | 358 |
| Poly(butyl chloroacrylate) | <chem>C=C(Cl)C(=O)OCCCC</chem> | 330 |
| Poly(butyl acrylate) | <chem>C=CC(=O)OCCCC</chem> | 219 |
| Poly(biphenyl-4-yl methacrylate) | <chem>C=C(C)C(=O)Oc2ccc(c1ccccc1)cc2</chem> | 413 |
| Poly(biphenyl-4-yl acrylate) | <chem>C=CC(=O)Oc2ccc(c1ccccc1)cc2</chem> | 383 |
| Poly(biphenyl-4-yl 2-methacrylate) | <chem>C=C(C)C(=O)Oc2cccc(c1ccccc1)c2</chem> | 413 |
| Poly(biphenyl-2-yl acrylate) | <chem>C=CC(=O)Oc1ccccc1c2ccccc2</chem> | 378 |
| Poly(benzyl methacrylate) | <chem>C=C(C)C(=O)OCc1ccccc1</chem> | 327 |
| Poly(benzyl acrylate) | <chem>C=CC(=O)OCc1ccccc1</chem> | 279 |
| Poly(acrylamide) | <chem>C=CC(N)=O</chem> | 438 |
| Poly(8-cyano-7-thiaoctyl acrylate) | <chem>C=CC(=O)OCCCCCSCC#N</chem> | 223 |
| Poly(6-cyano-4-thiahexyl acrylate) | <chem>C=CC(=O)OCCCSCCC#N</chem> | 215 |
| Poly(5-thiahexyl acrylate) | <chem>C=CC(=O)OCCCCSC</chem> | 203 |
| Poly(5-cyano-3-thiapentyl acrylate) | <chem>C=CC(=O)OCCSCCC#N</chem> | 214 |
| Poly(5-cyano-3-oxapentyl acrylate) | <chem>C=CC(=O)OCCCC(=O)CCC#N</chem> | 250 |
| Poly(5,5,6,6,7,7,7-heptafluoro-3-oxaheptyl acrylate) | <chem>C=CC(=O)OCCCC(=O)CC(F)(F)C(F)(F)C(F)(F)F</chem> | 228 |
| Poly(5,5,5-trifluoro-3-oxapentyl acrylate) | <chem>C=CC(=O)OCCCC(=O)CC(F)(F)F</chem> | 235 |
| Poly(4-thiahexyl acrylate) | <chem>C=CC(=O)OCCCSCC</chem> | 197 |
| Poly(4-terbutylphenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccc(C(C)(C)C)cc1</chem> | 371 |
| Poly(4-terbutylphenyl acrylate) | <chem>C=CC(=O)Oc1ccc(C(C)(C)C)cc1</chem> | 344 |
| Poly(4-methylphenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccc(C)cc1</chem> | 403 |
| Poly(4-methylphenyl acrylate) | <chem>C=CC(=O)Oc1ccc(C)cc1</chem> | 316 |
| Poly(4-methoxyphenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccc(OC)cc1</chem> | 379 |
| Poly(4-methoxyphenyl acrylate) | <chem>C=CC(=O)Oc1ccc(OC)cc1</chem> | 324 |
| Poly(4-cyanophenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccc(C#N)cc1</chem> | 428 |
| Poly(4-cyanophenyl acrylate) | <chem>C=CC(=O)Oc1ccc(C#N)cc1</chem> | 363 |
| Poly(4-cyanobutyl acrylate) | <chem>C=CC(=O)OCCCCC#N</chem> | 233 |
| Poly(4-cyanobenzyl acrylate) | <chem>C=CC(=O)OCc1ccc(C#N)cc1</chem> | 317 |
| Poly(4-cyano-3-thiabutyl acrylate) | <chem>C=CC(=O)OCCSCC#N</chem> | 249 |
| Poly(4-chlorophenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccc(Cl)cc1</chem> | 404 |
| Poly(4-chlorophenyl acrylate) | <chem>C=CC(=O)Oc1ccc(Cl)cc1</chem> | 330 |
| Poly(4-benzoylphenyl methacrylate) | <chem>C=C(C)C(=O)Oc2ccc(c1ccccc1)cc2</chem> | 391 |
| Poly(4,4,5,5-tetrafluoro-3-oxapentyl acrylate) | <chem>C=CC(=O)OCCCC(=O)C(F)(F)C(F)F</chem> | 251 |
| Poly(3-thiapentyl acrylate) | <chem>C=CC(=O)OCCSCC</chem> | 202 |
| Poly(3-thiabutyl acrylate) | <chem>C=CC(=O)OCCSC</chem> | 213 |
| Poly(3-oxa-butyl methacrylate) | <chem>C=C(C)C(=O)CCC(C)=O</chem> | 289 |
| Poly(3-oxa-5-hydroxypentyl methacrylate) | <chem>C=C(C)C(=O)CCC(=O)CCO</chem> | 278 |
| Poly(3-methylphenyl methacrylate) | <chem>C=C(C)C(=O)Oc1cccc(C)c1</chem> | 380 |

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| Poly(3-methylphenyl acrylate) | <chem>C=CC(=O)Oc1cccc(C)c1</chem> | 298 |
| Poly(3-methylbutyl acrylate) | <chem>C=CC(=O)OCCCC(C)C</chem> | 228 |
| Poly(3-methoxypropyl acrylate) | <chem>C=CC(=O)OCCCCOC</chem> | 198 |
| Poly(3-methoxyphenyl methacrylate) | <chem>C=C(C)C(=O)Oc1cccc(OC)c1</chem> | 343 |
| Poly(3-methoxybutyl acrylate) | <chem>C=CC(=O)OCCCC(C)OC</chem> | 217 |
| Poly(3-ethoxypropyl acrylate) | <chem>C=CC(=O)OCCCCOCC</chem> | 218 |
| Poly(3-dimethylaminophenyl acrylate) | <chem>C=CC(=O)Oc1cccc(N(C)C)c1</chem> | 320 |
| Poly(3-chlorophenyl acrylate) | <chem>C=CC(=O)Oc1cccc(Cl)c1</chem> | 312 |
| Poly(3,5,5-trimethylhexyl methacrylate) | <chem>C=C(C)C(=O)CCC(C)CC(C)(C)C</chem> | 274 |
| Poly(3,4-dimethylphenyl methylacrylate) | <chem>C=C(C)C(=O)Oc1ccc(C)c(C)c1</chem> | 384 |
| Poly(3,4-dimethylphenyl 2-methylacrylate) | <chem>C=C(C)C(=O)Oc1ccc(C)c(C)c1</chem> | 384 |
| Poly(3,3-dimethylbutyl methacrylate) | <chem>C=C(C)C(=O)OCCCC(C)(C)C</chem> | 318 |
| Poly(3,3-dimethyl-2-butylbutyl methacrylate) | <chem>C=C(C)C(=O)CC(CCCC)C(C)(C)C</chem> | 381 |
| Poly(2-terbutylphenyl acrylate) | <chem>C=CC(=O)Oc1cccc1C(C)(C)C</chem> | 345 |
| Poly(2-terbutylaminoethyl methacrylate) | <chem>C=C(C)C(=O)OCCNC(C)(C)C</chem> | 306 |
| Poly(2-phenylethyl methacrylate) | <chem>C=C(C)C(=O)OCCc1ccccc1</chem> | 299 |
| Poly(2-phenylethyl acrylate) | <chem>C=CC(=O)OCCc1ccccc1</chem> | 270 |
| Poly(2-octyl acrylate) | <chem>C=CC(=O)OC(C)CCCCC</chem> | 228 |
| Poly(2-methylphenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccccc1C</chem> | 382 |
| Poly(2-methylphenyl acrylate) | <chem>C=CC(=O)Oc1ccccc1C</chem> | 325 |
| Poly(2-methylpentyl acrylate) | <chem>C=CC(=O)OCC(C)CCC</chem> | 235 |
| Poly(2-methylbutyl acrylate) | <chem>C=CC(=O)OCC(C)CC</chem> | 241 |
| Poly(2-methoxyethyl acrylate) | <chem>C=CC(=O)OCCOC</chem> | 223 |
| Poly(2-hydroxyethyl methacrylate) | <chem>C=C(C)C(=O)CCO</chem> | 359 |
| Poly(2-heptyl acrylate) | <chem>C=CC(=O)OC(C)CCCCC</chem> | 235 |
| Poly(2-ethylhexyl methacrylate) | <chem>C=C(C)C(=O)CC(CC)CCCC</chem> | 263 |
| Poly(2-ethylbutyl methacrylate) | <chem>C=C(C)C(=O)CC(CC)CC</chem> | 284 |
| Poly(2-ethylbutyl acrylate) | <chem>C=CC(=O)OCC(CC)CC</chem> | 223 |
| Poly(2-ethoxyethyl acrylate) | <chem>C=CC(=O)OCCOCC</chem> | 223 |
| Poly(2-cyanoisopropyl acrylate) | <chem>C=CC(=O)OC(C)(C)C#N</chem> | 339 |
| Poly(2-cyanoisobutyl acrylate) | <chem>C=CC(=O)OCC(C)(C)C#N</chem> | 324 |
| Poly(2-cyanoethyl acrylate) | <chem>C=CC(=O)OCC(C#N)CCCC</chem> | 358 |
| Poly(2-cyanoheptyl acrylate) | <chem>C=CC(=O)OCC(C#N)CCCCC</chem> | 389 |
| Poly(2-cyanoethyl methacrylate) | <chem>C=C(C)C(=O)CCC#N</chem> | 364 |
| Poly(2-cyanoethyl acrylate) | <chem>C=CC(=O)OCCC#N</chem> | 277 |
| Poly(2-cyanobutyl acrylate) | <chem>C=CC(=O)OCC(C#N)CC</chem> | 384 |
| Poly(2-chloroethyl methacrylate) | <chem>C=C(C)C(=O)CCCl</chem> | 365 |
| Poly(2,4-dimethylphenyl methylacrylate) | <chem>C=C(C)C(=O)Oc1ccc(C)cc1C</chem> | 384 |
| Poly(2,4-dichlorophenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccc(Cl)cc1Cl</chem> | 391 |
| Poly(2,4-dichlorophenyl acrylate) | <chem>C=CC(=O)Oc1ccc(Cl)cc1Cl</chem> | 333 |
| Poly(2,3-dimethylphenyl methylacrylate) | <chem>C=C(C)C(=O)Oc1cccc(C)c1C</chem> | 398 |
| Poly(2,3-dimethylphenyl 2-methylacrylate) | <chem>C=C(C)C(=O)Oc1cccc(C)c1C</chem> | 398 |
| Poly(2,2,3,3,5,5,5-heptafluoro-4-oxapentyl acrylate) | <chem>C=CC(=O)OCC(F)(F)C(F)(F)C(=O)C(F)(F)F</chem> | 218 |
| Poly(2,2,2-trifluoroethyl acrylate) | <chem>C=CC(=O)OCC(F)(F)F</chem> | 263 |
| Poly(1H,1H-undecafluorohexyl acrylate) | <chem>C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F</chem> | 234 |
| Poly(1H,1H-undecafluoro-4-oxaheptyl acrylate) | <chem>C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(=O)C(F)(F)C(F)(F)F</chem> | 205 |
| Poly(1H,1H-nonafluoropentyl acrylate) | <chem>C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F</chem> | 236 |
| Poly(1H,1H-heptafluorobutyl acrylate) | <chem>C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)F</chem> | 243 |

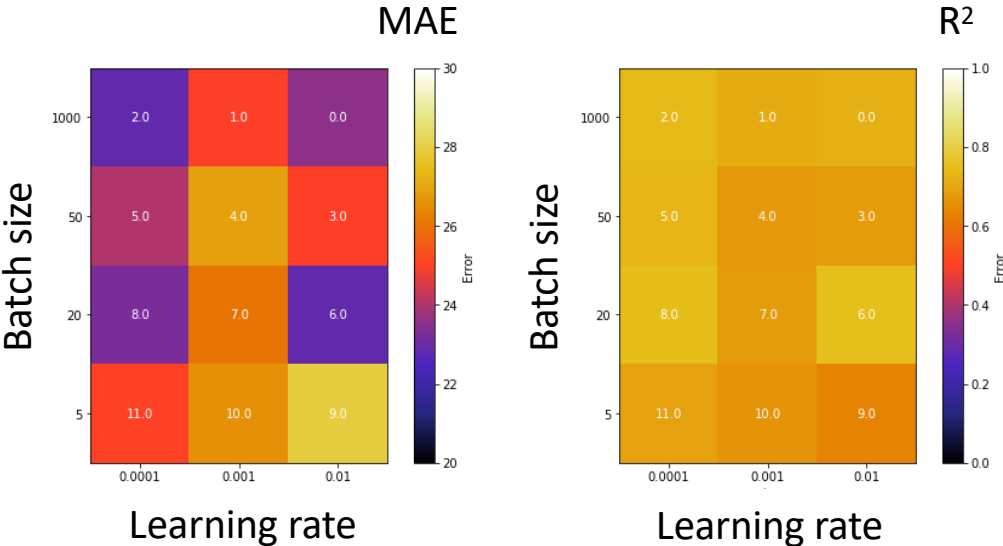
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| Poly(1H,1H,9H-hexadecafluorononyl methacrylate) | C=C(C)C(=O)CC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F) C(F)F | 258 |
| Poly(1H,1H,5H-octafluoropentyl methacrylate) | C=C(C)C(=O)CC(F)(F)C(F)(F)C(F)(F)C(F)F | 309 |
| Poly(1H,1H,5H-octafluoropentyl acrylate) | C=CC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F | 238 |
| Poly(1H,1H,3H-hexafluorobutyl acrylate) | C=CC(=O)OCC(F)(F)C(F)C(F)(F)F | 251 |
| Poly(1,3-dimethylbutyl acrylate) | C=CC(=O)OCC(C)C(C)C | 258 |
| Poly [methyl 3-(methacryloyloxy)benzoate] | C=C(C)C(=O)Oc1cccc(C(=O)OC)c1 | 345 |
| Poly [methyl 2-(methacryloyloxy)benzoate] | C=C(C)C(=O)Oc1ccccc1C(=O)OC | 337 |
| Poly [8-(4-(4-cyanophenyldiazenyl)phenoxy)octyl meth- acrylate] | C=CC(=O)OCCCCCCCc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 308 |
| Poly [6-(4-(4-nitrophenyldiazenyl)phenoxy)hexyl acry- late] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(N(=O)=O)cc1)cc2 | 309 |
| Poly [6-(4-(4-methoxyphenyldiazenyl)phenoxy)hexyl methacrylate] | C=C(C)C(=O)OCCCCCc2ccc(/N=N/c1ccc(OC)cc1)cc2 | 341 |
| Poly [6-(4-(4-methoxyphenyldiazenyl)phenoxy)hexyl acrylate] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(OC)cc1)cc2 | 319 |
| Poly [6-(4-(4-dimethylaminophenyldiazenyl)phe- noxy)hexyl methacrylate] | C=C(C)C(=O)OCCCCCc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2 | 359 |
| Poly [6-(4-(4-dimethylaminophenyl)diazanyl)phe- noxy]hexyl acrylate] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2 | 327 |
| Poly [6-(4-(4-cyanophenyldiazenyl)phenoxy)hexyl meth- acrylate] | C=C(C)C(=O)OCCCCCc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 333 |
| Poly [6-(4-(4-cyanophenyldiazenyl)phenoxy)hexyl acry- late] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 300 |
| Poly [6-(4-(4-butoxyphenyldiazenyl)phenoxy)hexyl methacrylate] | C=C(C)C(=O)OCCCCCc2ccc(/N=N/c1ccc(OCCCC)cc1)cc2 | 352 |
| Poly [6-((biphenyl-4-yl)oxy)hexyl acrylate] | C=CC(=O)OCCCCCc2ccc(c1ccccc1)cc2 | 321 |
| Poly [6-((4'-methoxybiphenyl-4-yl)oxy)hexyl acrylate] | C=CC(=O)OCCCCCc2ccc(c1ccc(OC)cc1)cc2 | 338 |
| Poly [6-((4'-cyanobiphenyl-4-yl)oxy)hexyl acrylate] | C=CC(=O)OCCCCCc2ccc(c1ccc(C#N)cc1)cc2 | 315 |
| Poly [5-((4'-cyanobiphenyl-4-yl)oxy)pentyl methacrylate] | C=C(C)C(=O)OCCCCCc2ccc(c1ccc(C#N)cc1)cc2 | 333 |
| Poly [5-((4'-cyanobiphenyl-4-yl)oxy)pentyl acrylate] | C=CC(=O)OCCCCCc2ccc(c1ccc(C#N)cc1)cc2 | 313 |
| Poly [4-(phenyldiazenyl)phenyl methacrylate] | C=C(C)C(=O)Oc2ccc(/N=N/c1ccccc1)cc2 | 374 |
| Poly [4-(4-dimethylaminophenyldiazenyl)phenyl methac- rylate] | C=C(C)C(=O)Oc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2 | 457 |
| Poly [4-(4-dimethylaminophenyldiazenyl)phenyl acry- late] | C=CC(=O)Oc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2 | 392 |
| Poly [4-(4-cyanophenyldiazenyl)phenyl methacrylate] | C=C(C)C(=O)Oc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 363 |
| Poly [4-(4-(4-nitrophenyldiazenyl)phenoxy)butyl acry- late] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(N(=O)=O)cc1)cc2 | 310 |
| Poly [4-(4-(4-cyanophenyldiazenyl)phenoxy)butyl meth- acrylate] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 353 |
| Poly [4-(3-methoxy-3-oxopropyl)phenyl methacrylate] | C=C(C)C(=O)Oc1ccc(CCC(=O)OC)cc1 | 341 |
| Poly [4-(2-methoxy-2-oxoethyl)phenyl methacrylate] | C=C(C)C(=O)Oc1ccc(CC(=O)OC)cc1 | 354 |
| Poly [3-(4-(4-nitrophenyldiazenyl)phenoxy)propyl acry- late] | C=CC(=O)OCCCCCc2ccc(/N=N/c1ccc(N(=O)=O)cc1)cc2 | 319 |
| Poly [2-(4-terbutylphenoxy)-2-oxoethyl methacrylate] | C=C(C)C(=O)OCC(=O)Oc1ccc(C(C)(C)C)cc1 | 368 |
| Poly [2-(4-(phenyldiazenyl)phenoxy)ethyl methacrylate] | C=C(C)C(=O)OCCOc2ccc(/N=N/c1ccccc1)cc2 | 378 |
| Poly [2-(4-(4-pentiloxypenyldiazenyl)-2-methylphe- noxy)hexyl acrylate] | CCCCCOc2ccc(/N=N/c1ccc(OCCCCCOC(C)=O)c(C)c1)cc2 | 294 |
| Poly [2-(2-(2-(2-(4-cyanophenyldiazenyl)phenoxy)eth- oxy)ethoxy)ethyl methacrylate] | C=C(C)C(=O)OCCOCCOCCOCCOc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 293 |
| Poly [2-(2-(2-(4'-methoxybiphenyl-4-yl)oxy)ethoxy)eth- oxy]ethyl acrylate] | C=CC(=O)OCCOCCOCCOc2ccc(c1ccc(OC)cc1)cc2 | 344 |
| Poly [2-(2-(2-(4-cyanophenyldiazenyl)phenoxy)eth- oxy)ethoxy]ethyl methacrylate] | C=C(C)C(=O)OCCOCCOCCOc2ccc(/N=N/c1ccc(C#N)cc1)cc2 | 310 |
| Poly [2-(2-(4-cyanophenyldiazenyl)phenoxy)eth- oxy]ethyl methacrylate] | C=C(C)C(=O)OCCOCCOc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2 | 314 |
| Poly [2-((4'-methoxybiphenyl-4-yl)oxy)ethyl acrylate] | C=CC(=O)OCOc2ccc(c1ccc(OC)cc1)cc2 | 353 |
| Poly [2-((4'-cyanobiphenyl-4-yl)oxy)ethyl methacrylate] | C=C(C)C(=O)OCCOc2ccc(c1ccc(C#N)cc1)cc2 | 368 |

| | | |
|---|--|-----|
| Poly [2-((4'-cyanobiphenyl-4-yl)oxy)ethyl acrylate] | <chem>C=CC(=O)OCCOc2ccc(c1ccc(C#N)cc1)cc2</chem> | 323 |
| Poly [11-(4'-(4'-cyanobiphenyl-4-yl)undecyl methacrylate] | <chem>C=C(C)C(=O)OCCCCCCCCCCCCc2ccc(c1ccc(C#N)cc1)cc2</chem> | 303 |
| Poly [11-(4-(4-(4-dimethylaminophenyldiazenyl)phenoxy)undecyl methacrylate] | <chem>C=C(C)C(=O)OCCCCCCCCCCCCOc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2</chem> | 344 |
| Poly [11-(4-(4-(4-dimethylaminophenyldiazenyl)phenoxy)undecyl acrylate] | <chem>C=CC(=O)OCCCCCCCCCCCCOc2ccc(/N=N/c1ccc(N(C)C)cc1)cc2</chem> | 321 |
| Poly [11-((4'-cyanobiphenyl-4-yl)oxy)undecyl methacrylate] | <chem>C=C(C)C(=O)OCCCCCCCCCCCCOc2ccc(c1ccc(C#N)cc1)cc2</chem> | 313 |
| Poly [11-((4'-cyanobiphenyl-4-yl)oxy)undecyl acrylate] | <chem>C=CC(=O)OCCCCCCCCCCCCOc2ccc(c1ccc(C#N)cc1)cc2</chem> | 303 |
| Poly [11-((4'-cyanobiphenyl-4-yl)oxy)-11-oxoundecyl methacrylate] | <chem>C=C(C)C(=O)OCCCCCCCCCCCCC(=O)Oc2ccc(c1ccc(C#N)cc1)cc2</chem> | 318 |
| Poly[ethyl 3-(acryloyloxy)benzoate] | <chem>C=CC(=O)Oc1cccc(C(=O)OCC)c1</chem> | 297 |
| Poly(propyl methacrylate) | <chem>C=C(C)C(=O)OCCC</chem> | 308 |
| Poly(propyl acrylate) | <chem>C=CC(=O)OCCC</chem> | 236 |
| Poly(octyl methacrylate) | <chem>C=C(C)C(=O)OCCCCCCCC</chem> | 253 |
| Poly(octyl acrylate) | <chem>C=CC(=O)OCCCCCCCC</chem> | 208 |
| Poly(2-chlorophenyl methacrylate) | <chem>C=C(C)C(=O)Oc1ccccc1Cl</chem> | 384 |
| Poly(2-chlorophenyl acrylate) | <chem>C=CC(=O)Oc1ccccc1Cl</chem> | 318 |
| Poly(1H,1H-pentafluoropropyl acrylate) | <chem>C=CC(=O)OCC(F)(F)C(F)(F)F</chem> | 247 |

b) Grid training DIRECT

Figure S1 shows grid training results (on external test) for the direct models. Mean average error (MAE) and R^2 as a function of learning rate and batch size are presented as colormaps for the 30 and 50% conditions.

TEST 30%



TEST 50%

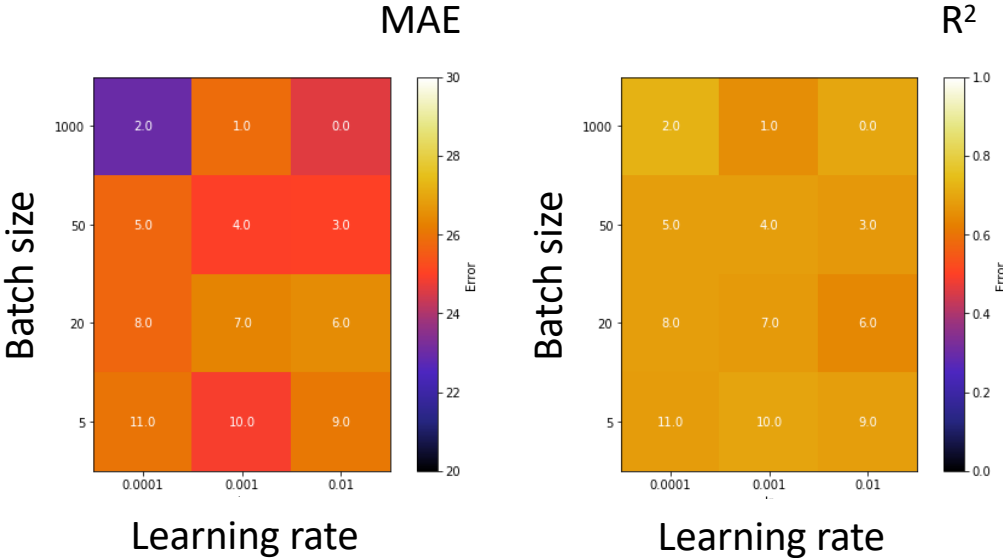


Figure S1

c) Predicted vs experimental results DIRECT

Figure S2 shows all corresponding “predicted vs experimental” results for 50% condition in direct models as hexbin plots. Each hexbin is coloured according to the mean relative deviation of the points within, and is numbered as in Figure S1.

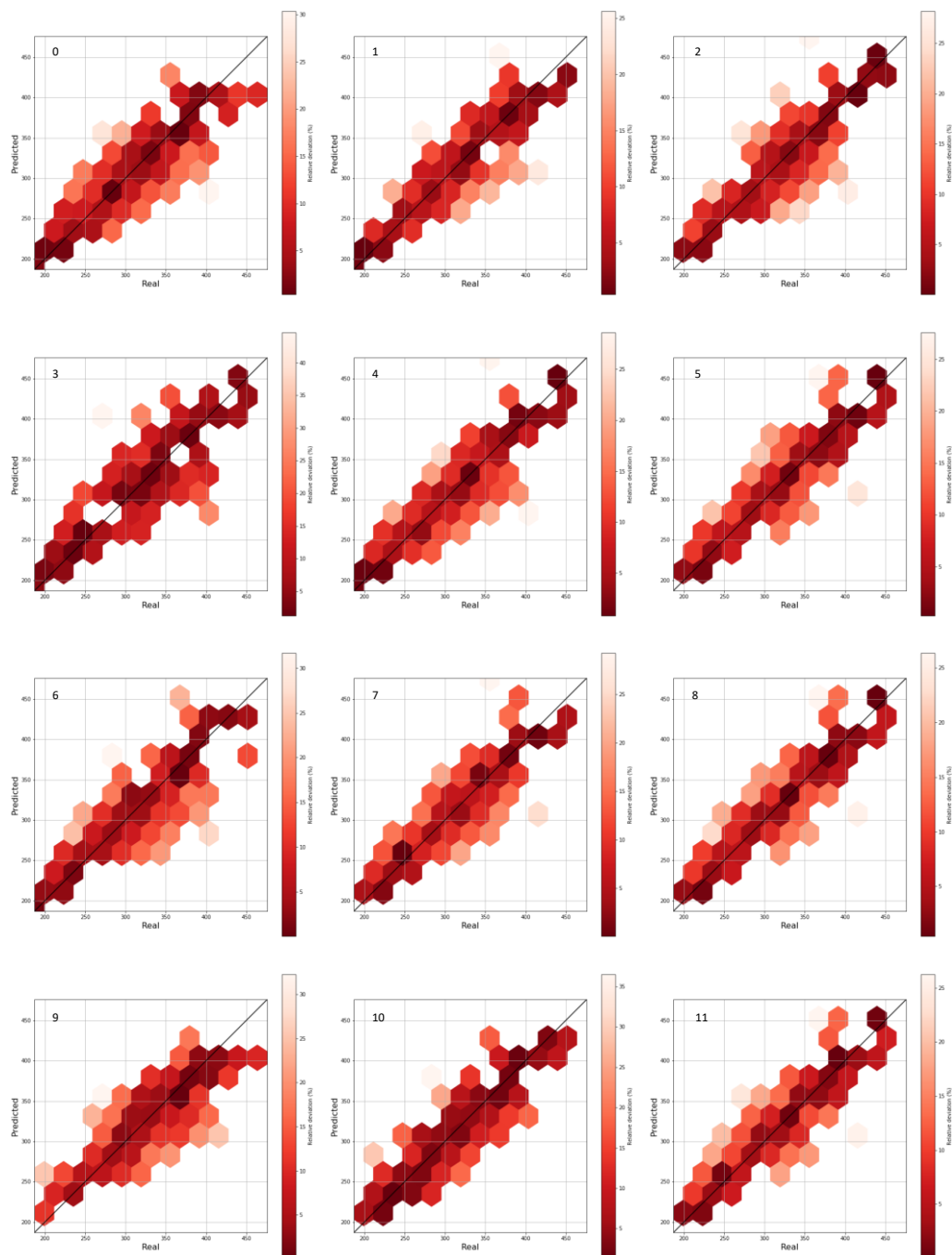
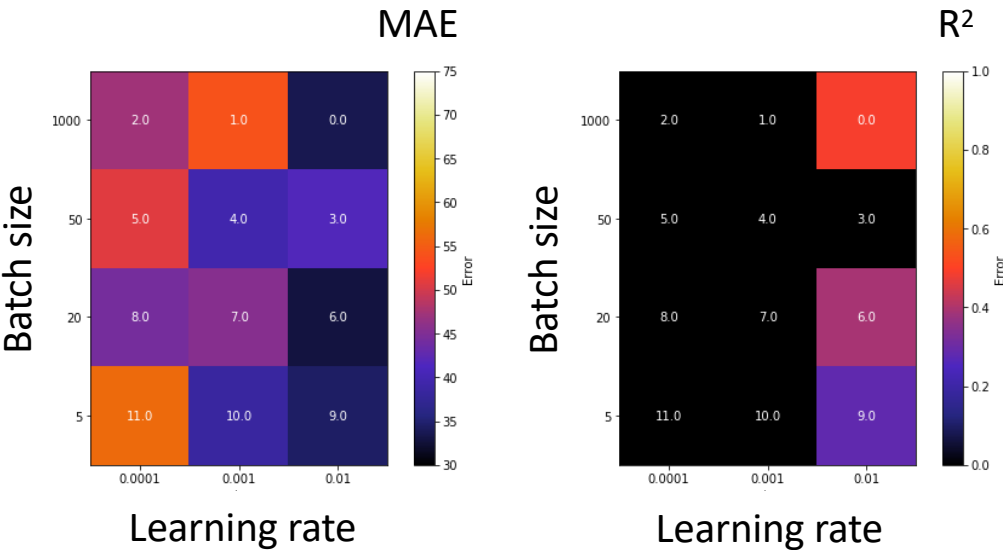


Figure S2

d) Grid training TL-based

Figure S3 shows grid training results (on external test) for the TL-based models. Mean average error (MAE) and R^2 as a function of learning rate and batch size are presented as colormaps for the 30 and 50% conditions.

TEST 30%



TEST 50%

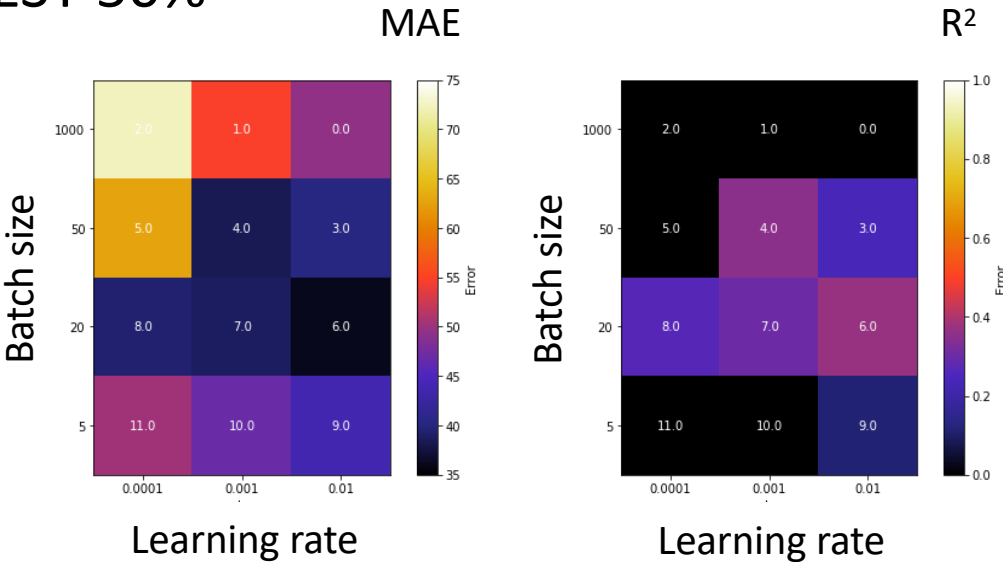


Figure S3

e) Predicted vs experimental results TL-based

Figure S4 shows all corresponding “predicted vs experimental” results for 50% condition in TL-based models as hexbin plots. Each hexbin is coloured according to the mean relative deviation of the points within, and is numbered as in Figure S3.

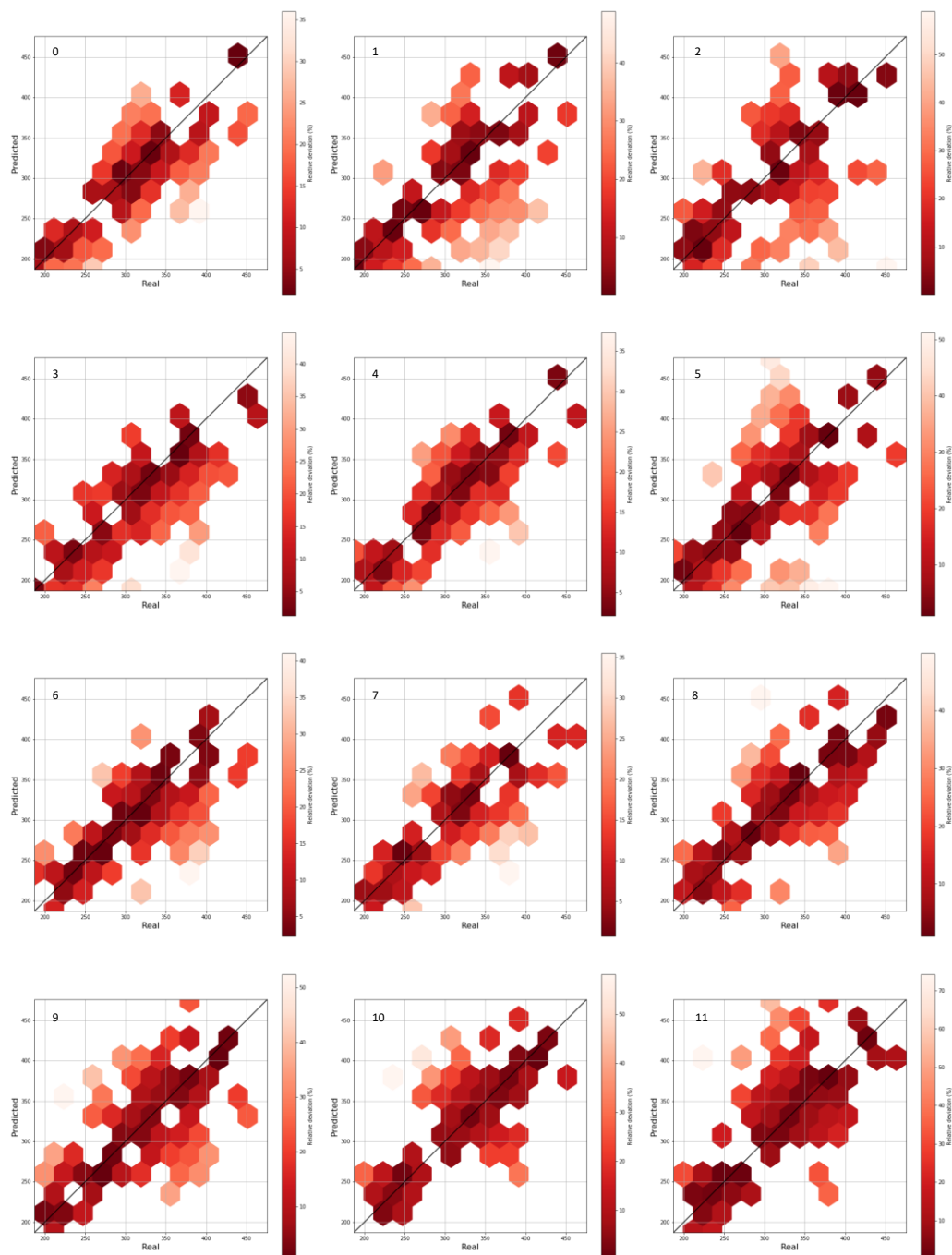


Figure S4