

targets :	cross_references ...	tax_id
0	[] ...	11119
1	[] ...	227859
2	[] ...	12663
3	[] ...	11137
4	[{'xref_id': 'P0C6U8', 'xref_name': None, 'xre...	227859
5	[] ...	1335626
6	[{'xref_id': 'P0C6X7', 'xref_name': None, 'xre...	227859
7	[] ...	2697049

11 [8 rows x 9 columns]

12 selected_target : CHEMBL3927

df2 :	activity_comment	activity_id	...	upper_value	value
0	None	1480935	...	None	7.2
1	None	1480936	...	None	9.4
2	None	1481061	...	None	13.5
3	None	1481065	...	None	13.11
4	None	1481066	...	None	2.0
..
128	None	12041507	...	None	10.6
129	None	12041508	...	None	10.1
130	None	12041509	...	None	11.5
131	None	12041510	...	None	10.7
132	None	12041511	...	None	78.9

26 [133 rows x 45 columns]

df3 :	molecule_chembl_id	...	standard_value
0	CHEMBL187579	...	7200.0
1	CHEMBL188487	...	9400.0
2	CHEMBL185698	...	13500.0
3	CHEMBL426082	...	13110.0
4	CHEMBL187717	...	2000.0
..
128	CHEMBL2146517	...	10600.0
129	CHEMBL187460	...	10100.0
130	CHEMBL363535	...	11500.0
131	CHEMBL227075	...	10700.0
132	CHEMBL45830	...	78900.0

40 [133 rows x 3 columns]

df4 :	molecule_chembl_id	...	bioactivity_class
0	CHEMBL187579	...	inactive
1	CHEMBL188487	...	inactive
2	CHEMBL185698	...	active
3	CHEMBL426082	...	active
4	CHEMBL187717	...	inactive
..
128	CHEMBL2146517	...	NaN
129	CHEMBL187460	...	NaN
130	CHEMBL363535	...	NaN
131	CHEMBL227075	...	NaN
132	CHEMBL45830	...	NaN

54 [133 rows x 4 columns]

55 adding: bioactivity_data_preprocessed.csv (deflated 80%)
56 adding: bioactivity_data_raw.csv (deflated 90%)
57 adding: mannwhitneyu_LogP.csv (deflated 9%)
58 adding: mannwhitneyu_MW.csv (deflated 8%)
59 adding: mannwhitneyu_NumHAcceptors.csv (deflated 10%)
60 adding: mannwhitneyu_NumHDonors.csv (deflated 10%)
61 adding: mannwhitneyu_pIC50.csv (deflated 11%)
62 adding: plot_bioactivity_class.pdf (deflated 38%)
63 adding: plot_ic50.pdf (deflated 37%)
64 adding: plot_LogP.pdf (deflated 38%)
65 adding: plot_MW.pdf (deflated 38%)
66 adding: plot_MW_vs_LogP.pdf (deflated 15%)
67 adding: plot_NumHAcceptors.pdf (deflated 37%)
68 adding: plot_NumHDonors.pdf (deflated 38%)
69 df_lipinski : MW LogP NumHDonors NumHAcceptors

```

70  0    281.271  1.89262      0.0      5.0
71  1    415.589  3.81320      0.0      2.0
72  2    421.190  2.66050      0.0      4.0
73  3    293.347  3.63080      0.0      3.0
74  4    338.344  3.53900      0.0      5.0
75  ..      ...      ...      ...      ...
76 128    338.359  3.40102      0.0      5.0
77 129    296.366  3.44330      0.0      3.0
78 130    276.291  4.09564      0.0      3.0
79 131    278.307  3.29102      0.0      3.0
80 132    282.383  4.10530      0.0      2.0
81
82 [133 rows x 4 columns]
83 df :      molecule_chembl_id  ... bioactivity_class
84  0      CHEMBL187579  ...      inactive
85  1      CHEMBL188487  ...      inactive
86  2      CHEMBL185698  ...      active
87  3      CHEMBL426082  ...      active
88  4      CHEMBL187717  ...      inactive
89  ..      ...      ...      ...
90 128      CHEMBL2146517  ...      NaN
91 129      CHEMBL187460  ...      NaN
92 130      CHEMBL363535  ...      NaN
93 131      CHEMBL227075  ...      NaN
94 132      CHEMBL45830  ...      NaN
95
96 [133 rows x 4 columns]
97 df_combined :      molecule_chembl_id  ... NumHAcceptors
98  0      CHEMBL187579  ...      5.0
99  1      CHEMBL188487  ...      2.0
100  2      CHEMBL185698  ...      4.0
101  3      CHEMBL426082  ...      3.0
102  4      CHEMBL187717  ...      5.0
103  ..      ...      ...      ...
104 128      CHEMBL2146517  ...      5.0
105 129      CHEMBL187460  ...      3.0
106 130      CHEMBL363535  ...      3.0
107 131      CHEMBL227075  ...      3.0
108 132      CHEMBL45830  ...      2.0
109
110 [133 rows x 8 columns]
111      molecule_chembl_id  ... standard_value_norm
112  0      CHEMBL187579  ...      7200.0
113  1      CHEMBL188487  ...      9400.0
114  2      CHEMBL185698  ...      13500.0
115  3      CHEMBL426082  ...      13110.0
116  4      CHEMBL187717  ...      2000.0
117  ..      ...      ...      ...
118 128      CHEMBL2146517  ...      10600.0
119 129      CHEMBL187460  ...      10100.0
120 130      CHEMBL363535  ...      11500.0
121 131      CHEMBL227075  ...      10700.0
122 132      CHEMBL45830  ...      78900.0
123
124 [133 rows x 8 columns]
125 df_final :      molecule_chembl_id  ...      pIC50
126  0      CHEMBL187579  ...      5.142668
127  1      CHEMBL188487  ...      5.026872
128  2      CHEMBL185698  ...      4.869666
129  3      CHEMBL426082  ...      4.882397
130  4      CHEMBL187717  ...      5.698970
131  ..      ...      ...      ...
132 128      CHEMBL2146517  ...      4.974694
133 129      CHEMBL187460  ...      4.995679
134 130      CHEMBL363535  ...      4.939302
135 131      CHEMBL227075  ...      4.970616
136 132      CHEMBL45830  ...      4.102923
137
138 [133 rows x 8 columns]

```

```

139 df_2class :      molecule_chembl_id ...      pIC50
140 0      CHEMBL187579 ... 5.142668
141 1      CHEMBL188487 ... 5.026872
142 2      CHEMBL185698 ... 4.869666
143 3      CHEMBL426082 ... 4.882397
144 4      CHEMBL187717 ... 5.698970
145 ..      ... ..
146 128     CHEMBL2146517 ... 4.974694
147 129     CHEMBL187460 ... 4.995679
148 130     CHEMBL363535 ... 4.939302
149 131     CHEMBL227075 ... 4.970616
150 132     CHEMBL45830 ... 4.102923
151
152 [133 rows x 8 columns]
153 mannwhitney('pIC50') :      Descriptor Statistics ... alpha
Interpretation
154 0      pIC50      588.0 ... 0.05 Same distribution (fail to reject H0)
155
156 [1 rows x 5 columns]
157 mannwhitney('MW') :      Descriptor Statistics ... alpha
Interpretation
158 0      MW      628.0 ... 0.05 Same distribution (fail to reject H0)
159
160 [1 rows x 5 columns]
161 mannwhitney('LogP') :      Descriptor Statistics ... alpha
Interpretation
162 0      LogP      608.0 ... 0.05 Same distribution (fail to reject H0)
163
164 [1 rows x 5 columns]
165 mannwhitney('NumHDonors') :      Descriptor Statistics ...
alpha Interpretation
166 0 NumHDonors      599.5 ... 0.05 Same distribution (fail to reject H0)
167
168 [1 rows x 5 columns]
169 mannwhitney('NumHAcceptors') :      Descriptor Statistics ...
alpha Interpretation
170 0 NumHAcceptors      726.0 ... 0.05 Same distribution (fail to reject H0)
171
172 [1 rows x 5 columns]
173 Archive: padel.zip
174 creating: PaDEL-Descriptor/
175 inflating: __MACOSX/._PaDEL-Descriptor
176 inflating: PaDEL-Descriptor/MACCSFingerprinter.xml
177 inflating: __MACOSX/PaDEL-Descriptor/._MACCSFingerprinter.xml
178 inflating: PaDEL-Descriptor/AtomPairs2DFingerprinter.xml
179 inflating: __MACOSX/PaDEL-Descriptor/._AtomPairs2DFingerprinter.xml
180 inflating: PaDEL-Descriptor/EStateFingerprinter.xml
181 inflating: __MACOSX/PaDEL-Descriptor/._EStateFingerprinter.xml
182 inflating: PaDEL-Descriptor/Fingerprinter.xml
183 inflating: __MACOSX/PaDEL-Descriptor/._Fingerprinter.xml
184 inflating: PaDEL-Descriptor/.DS_Store
185 inflating: __MACOSX/PaDEL-Descriptor/._.DS_Store
186 creating: PaDEL-Descriptor/license/
187 inflating: __MACOSX/PaDEL-Descriptor/._license
188 inflating: PaDEL-Descriptor/KlekotaRothFingerprintCount.xml
189 inflating: __MACOSX/PaDEL-Descriptor/._KlekotaRothFingerprintCount.xml
190 inflating: PaDEL-Descriptor/config
191 inflating: __MACOSX/PaDEL-Descriptor/._config
192 inflating: PaDEL-Descriptor/PubchemFingerprinter.xml
193 inflating: __MACOSX/PaDEL-Descriptor/._PubchemFingerprinter.xml
194 inflating: PaDEL-Descriptor/ExtendedFingerprinter.xml
195 inflating: __MACOSX/PaDEL-Descriptor/._ExtendedFingerprinter.xml
196 inflating: PaDEL-Descriptor/KlekotaRothFingerprinter.xml
197 inflating: __MACOSX/PaDEL-Descriptor/._KlekotaRothFingerprinter.xml
198 inflating: PaDEL-Descriptor/GraphOnlyFingerprinter.xml
199 inflating: __MACOSX/PaDEL-Descriptor/._GraphOnlyFingerprinter.xml
200 inflating: PaDEL-Descriptor/SubstructureFingerprinter.xml
201 inflating: __MACOSX/PaDEL-Descriptor/._SubstructureFingerprinter.xml
202 inflating: PaDEL-Descriptor/Descriptors.xls

```

203 inflating: __MACOSX/PaDEL-Descriptor/._Descriptors.xls
204 creating: PaDEL-Descriptor/lib/
205 inflating: __MACOSX/PaDEL-Descriptor/._lib
206 inflating: PaDEL-Descriptor/PaDEL-Descriptor.jar
207 inflating: __MACOSX/PaDEL-Descriptor/._PaDEL-Descriptor.jar
208 inflating: PaDEL-Descriptor/SubstructureFingerprintCount.xml
209 inflating: __MACOSX/PaDEL-Descriptor/._SubstructureFingerprintCount.xml
210 inflating: PaDEL-Descriptor/AtomPairs2DFingerprintCount.xml
211 inflating: __MACOSX/PaDEL-Descriptor/._AtomPairs2DFingerprintCount.xml
212 inflating: PaDEL-Descriptor/descriptors.xml
213 inflating: __MACOSX/PaDEL-Descriptor/._descriptors.xml
214 inflating: PaDEL-Descriptor/license/lgpl-2.1.txt
215 inflating: __MACOSX/PaDEL-Descriptor/license/._lgpl-2.1.txt
216 inflating: PaDEL-Descriptor/license/LICENSE.txt
217 inflating: __MACOSX/PaDEL-Descriptor/license/._LICENSE.txt
218 inflating: PaDEL-Descriptor/license/README - CDK
219 inflating: __MACOSX/PaDEL-Descriptor/license/._README - CDK
220 inflating: PaDEL-Descriptor/license/lgpl.license
221 inflating: __MACOSX/PaDEL-Descriptor/license/._lgpl.license
222 inflating: PaDEL-Descriptor/lib/ambit2-core-2.4.7-SNAPSHOT(3).jar
223 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-core-2.4.7-SNAPSHOT(3).jar
224 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(6).jar
225 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(6).jar
226 inflating: PaDEL-Descriptor/lib/libPaDEL.jar
227 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL.jar
228 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0(4).jar
229 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0(4).jar
230 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(2).jar
231 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(2).jar
232 inflating: PaDEL-Descriptor/lib/xom-1.1(1).jar
233 inflating: __MACOSX/PaDEL-Descriptor/lib/._xom-1.1(1).jar
234 inflating: PaDEL-Descriptor/lib/swing-worker-1.1.jar
235 inflating: __MACOSX/PaDEL-Descriptor/lib/._swing-worker-1.1.jar
236 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(3).jar
237 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(3).jar
238 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0(5).jar
239 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0(5).jar
240 inflating: PaDEL-Descriptor/lib/jama(1).jar
241 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(1).jar
242 inflating: PaDEL-Descriptor/lib/appframework-1.0.3.jar
243 inflating: __MACOSX/PaDEL-Descriptor/lib/._appframework-1.0.3.jar
244 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(7).jar
245 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(7).jar
246 inflating: PaDEL-Descriptor/lib/vecmath1.2-1.14.jar
247 inflating: __MACOSX/PaDEL-Descriptor/lib/._vecmath1.2-1.14.jar
248 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT(6).jar
249 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT(6).jar
250 inflating: PaDEL-Descriptor/lib/ambit2-core-2.4.7-SNAPSHOT(2).jar
251 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-core-2.4.7-SNAPSHOT(2).jar
252 inflating: PaDEL-Descriptor/lib/jama(6).jar
253 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(6).jar
254 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0(2).jar
255 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0(2).jar
256 inflating: PaDEL-Descriptor/lib/libPaDEL-Descriptor(3).jar
257 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Descriptor(3).jar
258 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(4).jar
259 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(4).jar
260 inflating: PaDEL-Descriptor/lib/ambit2-base-2.4.7-SNAPSHOT.jar
261 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-base-2.4.7-SNAPSHOT.jar
262 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT(1).jar
263 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT(1).jar
264 inflating: PaDEL-Descriptor/lib/commons-cli-1.2.jar
265 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2.jar
266 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(8).jar
267 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(8).jar
268 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0.jar
269 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0.jar
270 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(1).jar
271 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(1).jar

272 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs.jar
273 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs.jar
274 inflating: PaDEL-Descriptor/lib/ambit2-core-2.4.7-SNAPSHOT(4).jar
275 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-core-2.4.7-SNAPSHOT(4).jar
276 inflating: PaDEL-Descriptor/lib/xom-1.1.jar
277 inflating: __MACOSX/PaDEL-Descriptor/lib/._xom-1.1.jar
278 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(5).jar
279 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(5).jar
280 inflating: PaDEL-Descriptor/lib/libPaDEL-Descriptor(2).jar
281 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Descriptor(2).jar
282 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0(3).jar
283 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0(3).jar
284 inflating: PaDEL-Descriptor/lib/jama(7).jar
285 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(7).jar
286 inflating: PaDEL-Descriptor/lib/ambit2-core-2.4.7-SNAPSHOT.jar
287 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-core-2.4.7-SNAPSHOT.jar
288 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(6).jar
289 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(6).jar
290 inflating: PaDEL-Descriptor/lib/libPaDEL-Descriptor(1).jar
291 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Descriptor(1).jar
292 inflating: PaDEL-Descriptor/lib/jama(4).jar
293 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(4).jar
294 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(2).jar
295 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(2).jar
296 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT(3).jar
297 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT(3).jar
298 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT(2).jar
299 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT(2).jar
300 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT.jar
301 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT.jar
302 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(3).jar
303 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(3).jar
304 inflating: PaDEL-Descriptor/lib/l2fprod-common-all(1).jar
305 inflating: __MACOSX/PaDEL-Descriptor/lib/._l2fprod-common-all(1).jar
306 inflating: PaDEL-Descriptor/lib/jama.jar
307 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama.jar
308 inflating: PaDEL-Descriptor/lib/l2fprod-common-all.jar
309 inflating: __MACOSX/PaDEL-Descriptor/lib/._l2fprod-common-all.jar
310 inflating: PaDEL-Descriptor/lib/jama(5).jar
311 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(5).jar
312 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0(1).jar
313 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0(1).jar
314 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(7).jar
315 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(7).jar
316 inflating: PaDEL-Descriptor/lib/libPaDEL-Descriptor.jar
317 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Descriptor.jar
318 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(4).jar
319 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(4).jar
320 inflating: PaDEL-Descriptor/lib/cdk-1.4.15.jar
321 inflating: __MACOSX/PaDEL-Descriptor/lib/._cdk-1.4.15.jar
322 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT(5).jar
323 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT(5).jar
324 inflating: PaDEL-Descriptor/lib/ambit2-core-2.4.7-SNAPSHOT(1).jar
325 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-core-2.4.7-SNAPSHOT(1).jar
326 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(8).jar
327 inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(8).jar
328 inflating: PaDEL-Descriptor/lib/jgrapht-0.6.0(6).jar
329 inflating: __MACOSX/PaDEL-Descriptor/lib/._jgrapht-0.6.0(6).jar
330 inflating: PaDEL-Descriptor/lib/jama(2).jar
331 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(2).jar
332 inflating: PaDEL-Descriptor/lib/jama(3).jar
333 inflating: __MACOSX/PaDEL-Descriptor/lib/._jama(3).jar
334 inflating: PaDEL-Descriptor/lib/commons-cli-1.2(1).jar
335 inflating: __MACOSX/PaDEL-Descriptor/lib/._commons-cli-1.2(1).jar
336 inflating: PaDEL-Descriptor/lib/guava-17.0.jar
337 inflating: __MACOSX/PaDEL-Descriptor/lib/._guava-17.0.jar
338 inflating: PaDEL-Descriptor/lib/ambit2-smarts-2.4.7-SNAPSHOT(4).jar
339 inflating: __MACOSX/PaDEL-Descriptor/lib/._ambit2-smarts-2.4.7-SNAPSHOT(4).jar
340 inflating: PaDEL-Descriptor/lib/libPaDEL-Jobs(5).jar

```
341   inflating: __MACOSX/PaDEL-Descriptor/lib/._libPaDEL-Jobs(5).jar
342 4695
343 java -Xms1G -Xmx1G -Djava.awt.headless=true -jar
./PaDEL-Descriptor/PaDEL-Descriptor.jar -removesalt -standardizenitro -fingerprints
-descriptoratypes ./PaDEL-Descriptor/PubchemFingerprinter.xml -dir ./ -file
descriptors_output.csv
344 Processing CHEMBL130628 in molecule.smi (4/4695).
345 Processing CHEMBL133897 in molecule.smi (1/4695).
346 Processing CHEMBL336398 in molecule.smi (2/4695).
347 Processing CHEMBL131588 in molecule.smi (3/4695).
348 Processing CHEMBL130478 in molecule.smi (5/4695).
349 Processing CHEMBL130112 in molecule.smi (6/4695). Average speed: 5.90 s/mol.
350 Processing CHEMBL130098 in molecule.smi (7/4695). Average speed: 3.01 s/mol.
351 Processing CHEMBL337486 in molecule.smi (8/4695). Average speed: 1.52 s/mol.
352 Processing CHEMBL336538 in molecule.smi (9/4695). Average speed: 1.60 s/mol.
353 Processing CHEMBL131051 in molecule.smi (10/4695). Average speed: 1.39 s/mol.
354 Processing CHEMBL341437 in molecule.smi (11/4695). Average speed: 1.16 s/mol.
355 Processing CHEMBL335033 in molecule.smi (12/4695). Average speed: 1.01 s/mol.
356 Processing CHEMBL122983 in molecule.smi (13/4695). Average speed: 0.89 s/mol.
357 Processing CHEMBL338720 in molecule.smi (14/4695). Average speed: 0.82 s/mol.
358 Processing CHEMBL339995 in molecule.smi (15/4695). Average speed: 0.76 s/mol.
359 Processing CHEMBL335158 in molecule.smi (16/4695). Average speed: 0.71 s/mol.
360 Processing CHEMBL106126 in molecule.smi (18/4695). Average speed: 0.62 s/mol.
361 Processing CHEMBL131536 in molecule.smi (17/4695). Average speed: 0.66 s/mol.
362 Processing CHEMBL334971 in molecule.smi (19/4695). Average speed: 0.59 s/mol.
363 Processing CHEMBL336625 in molecule.smi (20/4695). Average speed: 0.55 s/mol.
364 Processing CHEMBL130666 in molecule.smi (21/4695). Average speed: 0.52 s/mol.
365 Processing CHEMBL134061 in molecule.smi (22/4695). Average speed: 0.51 s/mol.
366 Processing CHEMBL130645 in molecule.smi (24/4695). Average speed: 0.49 s/mol.
367 Processing CHEMBL133388 in molecule.smi (23/4695). Average speed: 0.48 s/mol.
368 Processing CHEMBL336524 in molecule.smi (26/4695). Average speed: 0.45 s/mol.
369 Processing CHEMBL336276 in molecule.smi (27/4695). Average speed: 0.45 s/mol.
370 Processing CHEMBL133580 in molecule.smi (25/4695). Average speed: 0.45 s/mol.
371 Processing CHEMBL334395 in molecule.smi (28/4695). Average speed: 0.39 s/mol.
372 Processing CHEMBL131320 in molecule.smi (29/4695). Average speed: 0.38 s/mol.
373 Processing CHEMBL339297 in molecule.smi (30/4695). Average speed: 0.37 s/mol.
374 Processing CHEMBL337714 in molecule.smi (31/4695). Average speed: 0.37 s/mol.
375 Processing CHEMBL122575 in molecule.smi (32/4695). Average speed: 0.35 s/mol.
376 Processing CHEMBL130704 in molecule.smi (33/4695). Average speed: 0.34 s/mol.
377 Processing CHEMBL46151 in molecule.smi (34/4695). Average speed: 0.33 s/mol.
378 Processing CHEMBL65667 in molecule.smi (37/4695). Average speed: 0.32 s/mol.
379 Processing CHEMBL297316 in molecule.smi (36/4695). Average speed: 0.33 s/mol.
380 Processing CHEMBL54126 in molecule.smi (35/4695). Average speed: 0.33 s/mol.
381 Processing CHEMBL431519 in molecule.smi (38/4695). Average speed: 0.30 s/mol.
382 Processing CHEMBL296429 in molecule.smi (39/4695). Average speed: 0.30 s/mol.
383 Processing CHEMBL154972 in molecule.smi (40/4695). Average speed: 0.29 s/mol.
384 Processing CHEMBL152722 in molecule.smi (41/4695). Average speed: 0.28 s/mol.
385 Processing CHEMBL544022 in molecule.smi (42/4695). Average speed: 0.28 s/mol.
386 Processing CHEMBL156659 in molecule.smi (44/4695). Average speed: 0.27 s/mol.
387 Processing CHEMBL349127 in molecule.smi (43/4695). Average speed: 0.27 s/mol.
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389 Processing CHEMBL45118 in molecule.smi (45/4695). Average speed: 0.26 s/mol.
390 Processing CHEMBL155322 in molecule.smi (47/4695). Average speed: 0.25 s/mol.
391 Processing CHEMBL154211 in molecule.smi (48/4695). Average speed: 0.25 s/mol.
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395 Processing CHEMBL345849 in molecule.smi (53/4695). Average speed: 0.24 s/mol.
396 Processing CHEMBL542360 in molecule.smi (52/4695). Average speed: 0.24 s/mol.
397 Processing CHEMBL154689 in molecule.smi (54/4695). Average speed: 0.23 s/mol.
398 Processing CHEMBL346733 in molecule.smi (55/4695). Average speed: 0.23 s/mol.
399 Processing CHEMBL416464 in molecule.smi (56/4695). Average speed: 0.22 s/mol.
400 Processing CHEMBL1203539 in molecule.smi (57/4695). Average speed: 0.22 s/mol.
401 Processing CHEMBL347729 in molecule.smi (58/4695). Average speed: 0.22 s/mol.
402 Processing CHEMBL296786 in molecule.smi (59/4695). Average speed: 0.21 s/mol.
403 Processing CHEMBL433041 in molecule.smi (61/4695). Average speed: 0.21 s/mol.
404 Processing CHEMBL63173 in molecule.smi (60/4695). Average speed: 0.21 s/mol.
405 Processing CHEMBL292788 in molecule.smi (62/4695). Average speed: 0.20 s/mol.
406 Processing CHEMBL33051 in molecule.smi (63/4695). Average speed: 0.20 s/mol.
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409 Processing CHEMBL543546 in molecule.smi (66/4695). Average speed: 0.20 s/mol.
410 Processing CHEMBL1420 in molecule.smi (67/4695). Average speed: 0.19 s/mol.
411 Processing CHEMBL556172 in molecule.smi (68/4695). Average speed: 0.19 s/mol.
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414 Processing CHEMBL155111 in molecule.smi (72/4695). Average speed: 0.19 s/mol.
415 Processing CHEMBL62664 in molecule.smi (71/4695). Average speed: 0.19 s/mol.
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420 Processing CHEMBL64011 in molecule.smi (77/4695). Average speed: 0.18 s/mol.
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645 Processing CHEMBL128172 in molecule.smi (302/4695). Average speed: 0.12 s/mol.
646 Processing CHEMBL155128 in molecule.smi (304/4695). Average speed: 0.12 s/mol.
647 Processing CHEMBL157017 in molecule.smi (303/4695). Average speed: 0.12 s/mol.
648 Processing CHEMBL345847 in molecule.smi (305/4695). Average speed: 0.12 s/mol.
649 Processing CHEMBL158252 in molecule.smi (306/4695). Average speed: 0.12 s/mol.
650 Processing CHEMBL341251 in molecule.smi (308/4695). Average speed: 0.12 s/mol.
651 Processing CHEMBL156874 in molecule.smi (307/4695). Average speed: 0.12 s/mol.
652 Processing CHEMBL445124 in molecule.smi (309/4695). Average speed: 0.12 s/mol.
653 Processing CHEMBL92142 in molecule.smi (310/4695). Average speed: 0.12 s/mol.
654 Processing CHEMBL553187 in molecule.smi (311/4695). Average speed: 0.12 s/mol.
655 Processing CHEMBL130956 in molecule.smi (312/4695). Average speed: 0.12 s/mol.
656 Processing CHEMBL93936 in molecule.smi (313/4695). Average speed: 0.12 s/mol.
657 Processing CHEMBL335167 in molecule.smi (314/4695). Average speed: 0.12 s/mol.
658 Processing CHEMBL92629 in molecule.smi (315/4695). Average speed: 0.12 s/mol.
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661 Processing CHEMBL93123 in molecule.smi (319/4695). Average speed: 0.12 s/mol.
662 Processing CHEMBL330004 in molecule.smi (318/4695). Average speed: 0.12 s/mol.
663 Processing CHEMBL420625 in molecule.smi (320/4695). Average speed: 0.11 s/mol.
664 Processing CHEMBL92460 in molecule.smi (321/4695). Average speed: 0.12 s/mol.
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666 Processing CHEMBL340391 in molecule.smi (322/4695). Average speed: 0.12 s/mol.
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674 Processing CHEMBL131825 in molecule.smi (332/4695). Average speed: 0.12 s/mol.
675 Processing CHEMBL335962 in molecule.smi (331/4695). Average speed: 0.12 s/mol.
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738 Processing CHEMBL176308 in molecule.smi (395/4695). Average speed: 0.12 s/mol.
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909 Processing CHEMBL358323 in molecule.smi (565/4695). Average speed: 0.11 s/mol.
910 Processing CHEMBL273904 in molecule.smi (567/4695). Average speed: 0.11 s/mol.
911 Processing CHEMBL137561 in molecule.smi (568/4695). Average speed: 0.11 s/mol.
912 Processing CHEMBL138988 in molecule.smi (569/4695). Average speed: 0.11 s/mol.
913 Processing CHEMBL136526 in molecule.smi (570/4695). Average speed: 0.11 s/mol.
914 Processing CHEMBL32768 in molecule.smi (571/4695). Average speed: 0.11 s/mol.
915 Processing CHEMBL145971 in molecule.smi (572/4695). Average speed: 0.11 s/mol.
916 Processing CHEMBL334938 in molecule.smi (574/4695). Average speed: 0.11 s/mol.
917 Processing CHEMBL352247 in molecule.smi (573/4695). Average speed: 0.11 s/mol.
918 Processing CHEMBL146158 in molecule.smi (575/4695). Average speed: 0.11 s/mol.
919 Processing CHEMBL345698 in molecule.smi (576/4695). Average speed: 0.11 s/mol.
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922 Processing CHEMBL58521 in molecule.smi (578/4695). Average speed: 0.11 s/mol.
923 Processing CHEMBL136294 in molecule.smi (581/4695). Average speed: 0.11 s/mol.
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925 Processing CHEMBL34000 in molecule.smi (582/4695). Average speed: 0.11 s/mol.
926 Processing CHEMBL347667 in molecule.smi (583/4695). Average speed: 0.11 s/mol.
927 Processing CHEMBL135086 in molecule.smi (585/4695). Average speed: 0.11 s/mol.
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929 Processing CHEMBL155191 in molecule.smi (587/4695). Average speed: 0.11 s/mol.
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1166 Processing CHEMBL541885 in molecule.smi (823/4695). Average speed: 0.09 s/mol.
1167 Processing CHEMBL147524 in molecule.smi (824/4695). Average speed: 0.09 s/mol.
1168 Processing CHEMBL147031 in molecule.smi (825/4695). Average speed: 0.09 s/mol.
1169 Processing CHEMBL544166 in molecule.smi (826/4695). Average speed: 0.09 s/mol.
1170 Processing CHEMBL359288 in molecule.smi (827/4695). Average speed: 0.09 s/mol.
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1173 Processing CHEMBL450931 in molecule.smi (830/4695). Average speed: 0.09 s/mol.
1174 Processing CHEMBL2093017 in molecule.smi (832/4695). Average speed: 0.09 s/mol.
1175 Processing CHEMBL358026 in molecule.smi (831/4695). Average speed: 0.09 s/mol.
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1178 Processing CHEMBL543216 in molecule.smi (835/4695). Average speed: 0.09 s/mol.
1179 Processing CHEMBL554056 in molecule.smi (837/4695). Average speed: 0.09 s/mol.
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1189 Processing CHEMBL554055 in molecule.smi (845/4695). Average speed: 0.09 s/mol.
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1211 Processing CHEMBL64633 in molecule.smi (868/4695). Average speed: 0.09 s/mol.
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1263 Processing CHEMBL362049 in molecule.smi (920/4695). Average speed: 0.10 s/mol.
1264 Processing CHEMBL178132 in molecule.smi (921/4695). Average speed: 0.10 s/mol.
1265 Processing CHEMBL361409 in molecule.smi (922/4695). Average speed: 0.10 s/mol.
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1295 Processing CHEMBL361869 in molecule.smi (952/4695). Average speed: 0.10 s/mol.
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1300 Processing CHEMBL191729 in molecule.smi (958/4695). Average speed: 0.10 s/mol.
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1302 Processing CHEMBL364125 in molecule.smi (959/4695). Average speed: 0.10 s/mol.
1303 Processing CHEMBL610243 in molecule.smi (960/4695). Average speed: 0.10 s/mol.

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1324	Processing	CHEMBL188714	in molecule.smi	(981/4695).	Average speed: 0.10 s/mol.
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1376 Processing CHEMBL557155 in molecule.smi (1033/4695). Average speed: 0.10 s/mol.
1377 Processing CHEMBL2113368 in molecule.smi (1035/4695). Average speed: 0.10 s/mol.
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1387 Processing CHEMBL371006 in molecule.smi (1044/4695). Average speed: 0.10 s/mol.
1388 Processing CHEMBL196177 in molecule.smi (1045/4695). Average speed: 0.10 s/mol.
1389 Processing CHEMBL196699 in molecule.smi (1046/4695). Average speed: 0.10 s/mol.
1390 Processing CHEMBL370561 in molecule.smi (1048/4695). Average speed: 0.10 s/mol.
1391 Processing CHEMBL371651 in molecule.smi (1047/4695). Average speed: 0.10 s/mol.
1392 Processing CHEMBL1385 in molecule.smi (1049/4695). Average speed: 0.10 s/mol.
1393 Processing CHEMBL194372 in molecule.smi (1050/4695). Average speed: 0.10 s/mol.
1394 Processing CHEMBL197696 in molecule.smi (1051/4695). Average speed: 0.10 s/mol.
1395 Processing CHEMBL199670 in molecule.smi (1052/4695). Average speed: 0.10 s/mol.
1396 Processing CHEMBL370807 in molecule.smi (1053/4695). Average speed: 0.10 s/mol.
1397 Processing CHEMBL372202 in molecule.smi (1054/4695). Average speed: 0.10 s/mol.
1398 Processing CHEMBL382260 in molecule.smi (1055/4695). Average speed: 0.10 s/mol.
1399 Processing CHEMBL199585 in molecule.smi (1056/4695). Average speed: 0.10 s/mol.
1400 Processing CHEMBL202661 in molecule.smi (1057/4695). Average speed: 0.10 s/mol.
1401 Processing CHEMBL381499 in molecule.smi (1058/4695). Average speed: 0.10 s/mol.
1402 Processing CHEMBL204895 in molecule.smi (1059/4695). Average speed: 0.10 s/mol.
1403 Processing CHEMBL382207 in molecule.smi (1060/4695). Average speed: 0.10 s/mol.
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1406 Processing CHEMBL381926 in molecule.smi (1063/4695). Average speed: 0.10 s/mol.
1407 Processing CHEMBL205940 in molecule.smi (1064/4695). Average speed: 0.10 s/mol.
1408 Processing CHEMBL205231 in molecule.smi (1065/4695). Average speed: 0.10 s/mol.
1409 Processing CHEMBL381782 in molecule.smi (1066/4695). Average speed: 0.10 s/mol.
1410 Processing CHEMBL205340 in molecule.smi (1067/4695). Average speed: 0.10 s/mol.
1411 Processing CHEMBL382351 in molecule.smi (1068/4695). Average speed: 0.10 s/mol.
1412 Processing CHEMBL205321 in molecule.smi (1069/4695). Average speed: 0.10 s/mol.
1413 Processing CHEMBL207777 in molecule.smi (1070/4695). Average speed: 0.10 s/mol.
1414 Processing CHEMBL378404 in molecule.smi (1071/4695). Average speed: 0.10 s/mol.
1415 Processing CHEMBL205967 in molecule.smi (1072/4695). Average speed: 0.10 s/mol.
1416 Processing CHEMBL380830 in molecule.smi (1073/4695). Average speed: 0.10 s/mol.
1417 Processing CHEMBL206093 in molecule.smi (1075/4695). Average speed: 0.10 s/mol.
1418 Processing CHEMBL206237 in molecule.smi (1074/4695). Average speed: 0.10 s/mol.
1419 Processing CHEMBL426674 in molecule.smi (1076/4695). Average speed: 0.10 s/mol.
1420 Processing CHEMBL377283 in molecule.smi (1077/4695). Average speed: 0.10 s/mol.
1421 Processing CHEMBL494887 in molecule.smi (1078/4695). Average speed: 0.10 s/mol.
1422 Processing CHEMBL464538 in molecule.smi (1079/4695). Average speed: 0.10 s/mol.
1423 Processing CHEMBL19224 in molecule.smi (1081/4695). Average speed: 0.10 s/mol.
1424 Processing CHEMBL383242 in molecule.smi (1080/4695). Average speed: 0.10 s/mol.
1425 Processing CHEMBL208132 in molecule.smi (1083/4695). Average speed: 0.10 s/mol.
1426 Processing CHEMBL207931 in molecule.smi (1082/4695). Average speed: 0.10 s/mol.
1427 Processing CHEMBL211383 in molecule.smi (1084/4695). Average speed: 0.10 s/mol.
1428 Processing CHEMBL211500 in molecule.smi (1085/4695). Average speed: 0.10 s/mol.
1429 Processing CHEMBL211450 in molecule.smi (1086/4695). Average speed: 0.10 s/mol.
1430 Processing CHEMBL212526 in molecule.smi (1087/4695). Average speed: 0.10 s/mol.
1431 Processing CHEMBL378763 in molecule.smi (1088/4695). Average speed: 0.10 s/mol.
1432 Processing CHEMBL378762 in molecule.smi (1089/4695). Average speed: 0.10 s/mol.
1433 Processing CHEMBL379950 in molecule.smi (1090/4695). Average speed: 0.10 s/mol.
1434 Processing CHEMBL212374 in molecule.smi (1091/4695). Average speed: 0.10 s/mol.
1435 Processing CHEMBL213281 in molecule.smi (1092/4695). Average speed: 0.10 s/mol.
1436 Processing CHEMBL379065 in molecule.smi (1093/4695). Average speed: 0.10 s/mol.
1437 Processing CHEMBL212001 in molecule.smi (1094/4695). Average speed: 0.10 s/mol.
1438 Processing CHEMBL212220 in molecule.smi (1095/4695). Average speed: 0.10 s/mol.
1439 Processing CHEMBL439508 in molecule.smi (1096/4695). Average speed: 0.10 s/mol.
1440 Processing CHEMBL213861 in molecule.smi (1097/4695). Average speed: 0.10 s/mol.
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1442 Processing CHEMBL212105 in molecule.smi (1099/4695). Average speed: 0.10 s/mol.
1443 Processing CHEMBL213240 in molecule.smi (1100/4695). Average speed: 0.10 s/mol.
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1448 Processing CHEMBL212377 in molecule.smi (1104/4695). Average speed: 0.10 s/mol.
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1451 Processing CHEMBL214160 in molecule.smi (1108/4695). Average speed: 0.10 s/mol.
1452 Processing CHEMBL213944 in molecule.smi (1109/4695). Average speed: 0.10 s/mol.
1453 Processing CHEMBL212771 in molecule.smi (1110/4695). Average speed: 0.10 s/mol.
1454 Processing CHEMBL211652 in molecule.smi (1111/4695). Average speed: 0.10 s/mol.
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1467 Processing CHEMBL386053 in molecule.smi (1123/4695). Average speed: 0.10 s/mol.
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1474 Processing CHEMBL211520 in molecule.smi (1131/4695). Average speed: 0.10 s/mol.
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1476 Processing CHEMBL384563 in molecule.smi (1133/4695). Average speed: 0.10 s/mol.
1477 Processing CHEMBL386541 in molecule.smi (1135/4695). Average speed: 0.10 s/mol.
1478 Processing CHEMBL415799 in molecule.smi (1134/4695). Average speed: 0.10 s/mol.
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1480 Processing CHEMBL219264 in molecule.smi (1137/4695). Average speed: 0.10 s/mol.
1481 Processing CHEMBL219316 in molecule.smi (1138/4695). Average speed: 0.10 s/mol.
1482 Processing CHEMBL384886 in molecule.smi (1139/4695). Average speed: 0.10 s/mol.
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1484 Processing CHEMBL445846 in molecule.smi (1141/4695). Average speed: 0.10 s/mol.
1485 Processing CHEMBL219911 in molecule.smi (1142/4695). Average speed: 0.10 s/mol.
1486 Processing CHEMBL374981 in molecule.smi (1143/4695). Average speed: 0.10 s/mol.
1487 Processing CHEMBL216159 in molecule.smi (1144/4695). Average speed: 0.10 s/mol.
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1498 Processing CHEMBL219400 in molecule.smi (1157/4695). Average speed: 0.10 s/mol.
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1503 Processing CHEMBL221811 in molecule.smi (1161/4695). Average speed: 0.10 s/mol.
1504 Processing CHEMBL266084 in molecule.smi (1160/4695). Average speed: 0.10 s/mol.
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1506 Processing CHEMBL221794 in molecule.smi (1163/4695). Average speed: 0.10 s/mol.
1507 Processing CHEMBL278193 in molecule.smi (1164/4695). Average speed: 0.10 s/mol.
1508 Processing CHEMBL376011 in molecule.smi (1165/4695). Average speed: 0.10 s/mol.
1509 Processing CHEMBL373674 in molecule.smi (1166/4695). Average speed: 0.10 s/mol.
1510 Processing CHEMBL220849 in molecule.smi (1168/4695). Average speed: 0.10 s/mol.

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1542 Processing CHEMBL225021 in molecule.smi (1199/4695). Average speed: 0.10 s/mol.
1543 Processing CHEMBL225610 in molecule.smi (1200/4695). Average speed: 0.10 s/mol.
1544 Processing CHEMBL224553 in molecule.smi (1201/4695). Average speed: 0.10 s/mol.
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1558 Processing CHEMBL225366 in molecule.smi (1215/4695). Average speed: 0.10 s/mol.
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1566 Processing CHEMBL427249 in molecule.smi (1223/4695). Average speed: 0.10 s/mol.
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1579 Processing CHEMBL244619 in molecule.smi (1236/4695). Average speed: 0.10 s/mol.

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1651 Processing CHEMBL241762 in molecule.smi (1308/4695). Average speed: 0.11 s/mol.
1652 Processing CHEMBL241761 in molecule.smi (1309/4695). Average speed: 0.11 s/mol.
1653 Processing CHEMBL392385 in molecule.smi (1310/4695). Average speed: 0.11 s/mol.
1654 Processing CHEMBL241760 in molecule.smi (1311/4695). Average speed: 0.11 s/mol.
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1657 Processing CHEMBL241552 in molecule.smi (1314/4695). Average speed: 0.11 s/mol.
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1660 Processing CHEMBL241548 in molecule.smi (1317/4695). Average speed: 0.11 s/mol.
1661 Processing CHEMBL397168 in molecule.smi (1318/4695). Average speed: 0.11 s/mol.
1662 Processing CHEMBL237189 in molecule.smi (1319/4695). Average speed: 0.11 s/mol.
1663 Processing CHEMBL392100 in molecule.smi (1320/4695). Average speed: 0.11 s/mol.
1664 Processing CHEMBL392099 in molecule.smi (1321/4695). Average speed: 0.11 s/mol.
1665 Processing CHEMBL238293 in molecule.smi (1322/4695). Average speed: 0.11 s/mol.
1666 Processing CHEMBL393149 in molecule.smi (1323/4695). Average speed: 0.11 s/mol.
1667 Processing CHEMBL438324 in molecule.smi (1325/4695). Average speed: 0.11 s/mol.
1668 Processing CHEMBL235761 in molecule.smi (1324/4695). Average speed: 0.11 s/mol.
1669 Processing CHEMBL235759 in molecule.smi (1326/4695). Average speed: 0.11 s/mol.
1670 Processing CHEMBL238257 in molecule.smi (1327/4695). Average speed: 0.11 s/mol.
1671 Processing CHEMBL238256 in molecule.smi (1328/4695). Average speed: 0.11 s/mol.
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1676 Processing CHEMBL238764 in molecule.smi (1333/4695). Average speed: 0.10 s/mol.
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1678 Processing CHEMBL239418 in molecule.smi (1335/4695). Average speed: 0.10 s/mol.
1679 Processing CHEMBL397160 in molecule.smi (1336/4695). Average speed: 0.10 s/mol.
1680 Processing CHEMBL239207 in molecule.smi (1337/4695). Average speed: 0.10 s/mol.
1681 Processing CHEMBL241127 in molecule.smi (1338/4695). Average speed: 0.10 s/mol.
1682 Processing CHEMBL1203985 in molecule.smi (1339/4695). Average speed: 0.10 s/mol.
1683 Processing CHEMBL555247 in molecule.smi (1341/4695). Average speed: 0.10 s/mol.
1684 Processing CHEMBL360055 in molecule.smi (1340/4695). Average speed: 0.10 s/mol.
1685 Processing CHEMBL1203984 in molecule.smi (1342/4695). Average speed: 0.10 s/mol.
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1692 Processing CHEMBL251077 in molecule.smi (1349/4695). Average speed: 0.11 s/mol.
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1694 Processing CHEMBL1524 in molecule.smi (1351/4695). Average speed: 0.11 s/mol.
1695 Processing CHEMBL251076 in molecule.smi (1352/4695). Average speed: 0.11 s/mol.
1696 Processing CHEMBL409610 in molecule.smi (1353/4695). Average speed: 0.11 s/mol.
1697 Processing CHEMBL400092 in molecule.smi (1355/4695). Average speed: 0.11 s/mol.
1698 Processing CHEMBL401114 in molecule.smi (1354/4695). Average speed: 0.11 s/mol.
1699 Processing CHEMBL250688 in molecule.smi (1356/4695). Average speed: 0.11 s/mol.
1700 Processing CHEMBL252723 in molecule.smi (1357/4695). Average speed: 0.11 s/mol.
1701 Processing CHEMBL1523 in molecule.smi (1358/4695). Average speed: 0.11 s/mol.
1702 Processing CHEMBL479291 in molecule.smi (1359/4695). Average speed: 0.11 s/mol.
1703 Processing CHEMBL15056 in molecule.smi (1360/4695). Average speed: 0.11 s/mol.
1704 Processing CHEMBL41 in molecule.smi (1361/4695). Average speed: 0.11 s/mol.
1705 Processing CHEMBL255231 in molecule.smi (1362/4695). Average speed: 0.11 s/mol.
1706 Processing CHEMBL109018 in molecule.smi (1364/4695). Average speed: 0.11 s/mol.
1707 Processing CHEMBL255230 in molecule.smi (1363/4695). Average speed: 0.11 s/mol.
1708 Processing CHEMBL257540 in molecule.smi (1365/4695). Average speed: 0.11 s/mol.
1709 Processing CHEMBL403260 in molecule.smi (1366/4695). Average speed: 0.11 s/mol.
1710 Processing CHEMBL254016 in molecule.smi (1367/4695). Average speed: 0.11 s/mol.
1711 Processing CHEMBL231160 in molecule.smi (1368/4695). Average speed: 0.11 s/mol.
1712 Processing CHEMBL32329 in molecule.smi (1369/4695). Average speed: 0.11 s/mol.
1713 Processing CHEMBL590603 in molecule.smi (1370/4695). Average speed: 0.11 s/mol.
1714 Processing CHEMBL270248 in molecule.smi (1371/4695). Average speed: 0.11 s/mol.
1715 Processing CHEMBL271710 in molecule.smi (1372/4695). Average speed: 0.11 s/mol.
1716 Processing CHEMBL271709 in molecule.smi (1373/4695). Average speed: 0.11 s/mol.
1717 Processing CHEMBL26125 in molecule.smi (1374/4695). Average speed: 0.11 s/mol.

1718 Processing CHEMBL407904 in molecule.smi (1375/4695). Average speed: 0.11 s/mol.
1719 Processing CHEMBL248922 in molecule.smi (1376/4695). Average speed: 0.11 s/mol.
1720 Processing CHEMBL239046 in molecule.smi (1377/4695). Average speed: 0.11 s/mol.
1721 Processing CHEMBL272700 in molecule.smi (1378/4695). Average speed: 0.11 s/mol.
1722 Processing CHEMBL269865 in molecule.smi (1379/4695). Average speed: 0.11 s/mol.
1723 Processing CHEMBL271385 in molecule.smi (1380/4695). Average speed: 0.11 s/mol.
1724 Processing CHEMBL271746 in molecule.smi (1381/4695). Average speed: 0.11 s/mol.
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1726 Processing CHEMBL260964 in molecule.smi (1383/4695). Average speed: 0.11 s/mol.
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2113 Processing CHEMBL141203 in molecule.smi (1771/4695). Average speed: 0.11 s/mol.
2114 Processing CHEMBL140106 in molecule.smi (1770/4695). Average speed: 0.11 s/mol.
2115 Processing CHEMBL142014 in molecule.smi (1772/4695). Average speed: 0.11 s/mol.
2116 Processing CHEMBL140990 in molecule.smi (1773/4695). Average speed: 0.11 s/mol.
2117 Processing CHEMBL142013 in molecule.smi (1774/4695). Average speed: 0.11 s/mol.
2118 Processing CHEMBL141042 in molecule.smi (1775/4695). Average speed: 0.11 s/mol.
2119 Processing CHEMBL140328 in molecule.smi (1776/4695). Average speed: 0.11 s/mol.
2120 Processing CHEMBL141810 in molecule.smi (1777/4695). Average speed: 0.11 s/mol.
2121 Processing CHEMBL342413 in molecule.smi (1778/4695). Average speed: 0.11 s/mol.
2122 Processing CHEMBL141276 in molecule.smi (1779/4695). Average speed: 0.11 s/mol.
2123 Processing CHEMBL138552 in molecule.smi (1780/4695). Average speed: 0.11 s/mol.
2124 Processing CHEMBL141515 in molecule.smi (1781/4695). Average speed: 0.11 s/mol.
2125 Processing CHEMBL1083069 in molecule.smi (1782/4695). Average speed: 0.11 s/mol.
2126 Processing CHEMBL129753 in molecule.smi (1783/4695). Average speed: 0.11 s/mol.
2127 Processing CHEMBL1083070 in molecule.smi (1784/4695). Average speed: 0.11 s/mol.
2128 Processing CHEMBL337999 in molecule.smi (1785/4695). Average speed: 0.11 s/mol.
2129 Processing CHEMBL1083379 in molecule.smi (1786/4695). Average speed: 0.11 s/mol.
2130 Processing CHEMBL128863 in molecule.smi (1787/4695). Average speed: 0.11 s/mol.
2131 Processing CHEMBL130847 in molecule.smi (1789/4695). Average speed: 0.11 s/mol.

2132 Processing CHEMBL336297 in molecule.smi (1788/4695). Average speed: 0.11 s/mol.
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2134 Processing CHEMBL131827 in molecule.smi (1791/4695). Average speed: 0.11 s/mol.
2135 Processing CHEMBL1084090 in molecule.smi (1793/4695). Average speed: 0.11 s/mol.
2136 Processing CHEMBL130918 in molecule.smi (1792/4695). Average speed: 0.11 s/mol.
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2138 Processing CHEMBL128551 in molecule.smi (1795/4695). Average speed: 0.11 s/mol.
2139 Processing CHEMBL1084883 in molecule.smi (1796/4695). Average speed: 0.11 s/mol.
2140 Processing CHEMBL128618 in molecule.smi (1797/4695). Average speed: 0.11 s/mol.
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2157 Processing CHEMBL278819 in molecule.smi (1814/4695). Average speed: 0.11 s/mol.
2158 Processing CHEMBL150985 in molecule.smi (1816/4695). Average speed: 0.11 s/mol.
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2163 Processing CHEMBL150365 in molecule.smi (1820/4695). Average speed: 0.11 s/mol.
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2180 Processing CHEMBL1084542 in molecule.smi (1837/4695). Average speed: 0.11 s/mol.
2181 Processing CHEMBL1084543 in molecule.smi (1838/4695). Average speed: 0.11 s/mol.
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2188 Processing CHEMBL1082435 in molecule.smi (1845/4695). Average speed: 0.11 s/mol.
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2190 Processing CHEMBL1084790 in molecule.smi (1847/4695). Average speed: 0.11 s/mol.
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2192 Processing CHEMBL100334 in molecule.smi (1849/4695). Average speed: 0.11 s/mol.
2193 Processing CHEMBL102142 in molecule.smi (1850/4695). Average speed: 0.11 s/mol.
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2195 Processing CHEMBL101518 in molecule.smi (1852/4695). Average speed: 0.11 s/mol.
2196 Processing CHEMBL430679 in molecule.smi (1853/4695). Average speed: 0.11 s/mol.
2197 Processing CHEMBL101940 in molecule.smi (1854/4695). Average speed: 0.11 s/mol.
2198 Processing CHEMBL101809 in molecule.smi (1855/4695). Average speed: 0.11 s/mol.
2199 Processing CHEMBL100510 in molecule.smi (1856/4695). Average speed: 0.11 s/mol.
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2204 Processing CHEMBL101988 in molecule.smi (1861/4695). Average speed: 0.11 s/mol.
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2236 Processing CHEMBL332454 in molecule.smi (1893/4695). Average speed: 0.11 s/mol.
2237 Processing CHEMBL119634 in molecule.smi (1894/4695). Average speed: 0.11 s/mol.
2238 Processing CHEMBL118139 in molecule.smi (1895/4695). Average speed: 0.11 s/mol.
2239 Processing CHEMBL117826 in molecule.smi (1896/4695). Average speed: 0.11 s/mol.
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2244 Processing CHEMBL119528 in molecule.smi (1900/4695). Average speed: 0.11 s/mol.
2245 Processing CHEMBL119389 in molecule.smi (1902/4695). Average speed: 0.11 s/mol.
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2247 Processing CHEMBL1083677 in molecule.smi (1904/4695). Average speed: 0.11 s/mol.
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2262 Processing CHEMBL91240 in molecule.smi (1919/4695). Average speed: 0.11 s/mol.
2263 Processing CHEMBL90264 in molecule.smi (1920/4695). Average speed: 0.11 s/mol.
2264 Processing CHEMBL91774 in molecule.smi (1922/4695). Average speed: 0.11 s/mol.
2265 Processing CHEMBL91432 in molecule.smi (1921/4695). Average speed: 0.11 s/mol.
2266 Processing CHEMBL421501 in molecule.smi (1923/4695). Average speed: 0.11 s/mol.
2267 Processing CHEMBL76014 in molecule.smi (1924/4695). Average speed: 0.11 s/mol.
2268 Processing CHEMBL74827 in molecule.smi (1925/4695). Average speed: 0.11 s/mol.
2269 Processing CHEMBL73800 in molecule.smi (1926/4695). Average speed: 0.11 s/mol.

2270 Processing CHEMBL75274 in molecule.smi (1927/4695). Average speed: 0.11 s/mol.
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2273 Processing CHEMBL312761 in molecule.smi (1930/4695). Average speed: 0.11 s/mol.
2274 Processing CHEMBL73160 in molecule.smi (1931/4695). Average speed: 0.11 s/mol.
2275 Processing CHEMBL307004 in molecule.smi (1932/4695). Average speed: 0.11 s/mol.
2276 Processing CHEMBL312310 in molecule.smi (1933/4695). Average speed: 0.11 s/mol.
2277 Processing CHEMBL75305 in molecule.smi (1934/4695). Average speed: 0.11 s/mol.
2278 Processing CHEMBL76173 in molecule.smi (1935/4695). Average speed: 0.11 s/mol.
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2293 Processing CHEMBL1085940 in molecule.smi (1950/4695). Average speed: 0.11 s/mol.
2294 Processing CHEMBL224158 in molecule.smi (1951/4695). Average speed: 0.11 s/mol.
2295 Processing CHEMBL224335 in molecule.smi (1952/4695). Average speed: 0.11 s/mol.
2296 Processing CHEMBL1083983 in molecule.smi (1953/4695). Average speed: 0.11 s/mol.
2297 Processing CHEMBL1083984 in molecule.smi (1954/4695). Average speed: 0.11 s/mol.
2298 Processing CHEMBL389192 in molecule.smi (1955/4695). Average speed: 0.11 s/mol.
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2314 Processing CHEMBL1084545 in molecule.smi (1971/4695). Average speed: 0.11 s/mol.
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2316 Processing CHEMBL185896 in molecule.smi (1973/4695). Average speed: 0.11 s/mol.
2317 Processing CHEMBL325109 in molecule.smi (1974/4695). Average speed: 0.11 s/mol.
2318 Processing CHEMBL362579 in molecule.smi (1975/4695). Average speed: 0.11 s/mol.
2319 Processing CHEMBL189870 in molecule.smi (1976/4695). Average speed: 0.11 s/mol.
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2323 Processing CHEMBL188019 in molecule.smi (1979/4695). Average speed: 0.11 s/mol.
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4001 Processing CHEMBL3781564 in molecule.smi (3658/4695). Average speed: 0.13 s/mol.
4002 Processing CHEMBL3780448 in molecule.smi (3659/4695). Average speed: 0.13 s/mol.
4003 Processing CHEMBL3780131 in molecule.smi (3660/4695). Average speed: 0.13 s/mol.
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4006 Processing CHEMBL3786544 in molecule.smi (3663/4695). Average speed: 0.13 s/mol.
4007 Processing CHEMBL3787307 in molecule.smi (3664/4695). Average speed: 0.13 s/mol.
4008 Processing CHEMBL3786666 in molecule.smi (3665/4695). Average speed: 0.13 s/mol.
4009 Processing CHEMBL3785481 in molecule.smi (3666/4695). Average speed: 0.13 s/mol.
4010 Processing CHEMBL3786655 in molecule.smi (3667/4695). Average speed: 0.13 s/mol.
4011 Processing CHEMBL3786447 in molecule.smi (3670/4695). Average speed: 0.13 s/mol.
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4013 Processing CHEMBL3785526 in molecule.smi (3668/4695). Average speed: 0.13 s/mol.
4014 Processing CHEMBL3787666 in molecule.smi (3671/4695). Average speed: 0.13 s/mol.
4015 Processing CHEMBL3785229 in molecule.smi (3672/4695). Average speed: 0.13 s/mol.
4016 Processing CHEMBL3785187 in molecule.smi (3673/4695). Average speed: 0.13 s/mol.
4017 Processing CHEMBL3785803 in molecule.smi (3674/4695). Average speed: 0.13 s/mol.
4018 Processing CHEMBL3786323 in molecule.smi (3675/4695). Average speed: 0.13 s/mol.
4019 Processing CHEMBL3786589 in molecule.smi (3676/4695). Average speed: 0.13 s/mol.
4020 Processing CHEMBL3786505 in molecule.smi (3677/4695). Average speed: 0.13 s/mol.
4021 Processing CHEMBL3785644 in molecule.smi (3678/4695). Average speed: 0.13 s/mol.
4022 Processing CHEMBL3785808 in molecule.smi (3679/4695). Average speed: 0.13 s/mol.
4023 Processing CHEMBL3786651 in molecule.smi (3680/4695). Average speed: 0.13 s/mol.
4024 Processing CHEMBL3786516 in molecule.smi (3681/4695). Average speed: 0.13 s/mol.
4025 Processing CHEMBL3787502 in molecule.smi (3682/4695). Average speed: 0.13 s/mol.
4026 Processing CHEMBL3785269 in molecule.smi (3683/4695). Average speed: 0.13 s/mol.
4027 Processing CHEMBL3787223 in molecule.smi (3684/4695). Average speed: 0.13 s/mol.
4028 Processing CHEMBL3786448 in molecule.smi (3685/4695). Average speed: 0.13 s/mol.
4029 Processing CHEMBL3786937 in molecule.smi (3686/4695). Average speed: 0.13 s/mol.
4030 Processing CHEMBL3785391 in molecule.smi (3687/4695). Average speed: 0.13 s/mol.
4031 Processing CHEMBL3786873 in molecule.smi (3689/4695). Average speed: 0.13 s/mol.
4032 Processing CHEMBL3785207 in molecule.smi (3688/4695). Average speed: 0.13 s/mol.
4033 Processing CHEMBL3786442 in molecule.smi (3690/4695). Average speed: 0.13 s/mol.
4034 Processing CHEMBL3809337 in molecule.smi (3692/4695). Average speed: 0.13 s/mol.
4035 Processing CHEMBL3786719 in molecule.smi (3691/4695). Average speed: 0.13 s/mol.
4036 Processing CHEMBL355160 in molecule.smi (3694/4695). Average speed: 0.13 s/mol.
4037 Processing CHEMBL1929043 in molecule.smi (3693/4695). Average speed: 0.13 s/mol.
4038 Processing CHEMBL3818415 in molecule.smi (3695/4695). Average speed: 0.13 s/mol.
4039 Processing CHEMBL3819155 in molecule.smi (3696/4695). Average speed: 0.13 s/mol.
4040 Processing CHEMBL3818230 in molecule.smi (3697/4695). Average speed: 0.13 s/mol.
4041 Processing CHEMBL3818616 in molecule.smi (3698/4695). Average speed: 0.13 s/mol.
4042 Processing CHEMBL3819646 in molecule.smi (3699/4695). Average speed: 0.13 s/mol.
4043 Processing CHEMBL168938 in molecule.smi (3700/4695). Average speed: 0.13 s/mol.
4044 Processing CHEMBL3819220 in molecule.smi (3701/4695). Average speed: 0.13 s/mol.
4045 Processing CHEMBL3818167 in molecule.smi (3702/4695). Average speed: 0.13 s/mol.
4046 Processing CHEMBL3818084 in molecule.smi (3703/4695). Average speed: 0.13 s/mol.
4047 Processing CHEMBL3818801 in molecule.smi (3704/4695). Average speed: 0.13 s/mol.
4048 Processing CHEMBL3819113 in molecule.smi (3706/4695). Average speed: 0.13 s/mol.
4049 Processing CHEMBL3819531 in molecule.smi (3705/4695). Average speed: 0.13 s/mol.
4050 Processing CHEMBL3819574 in molecule.smi (3707/4695). Average speed: 0.13 s/mol.
4051 Processing CHEMBL3819247 in molecule.smi (3708/4695). Average speed: 0.13 s/mol.
4052 Processing CHEMBL3819024 in molecule.smi (3710/4695). Average speed: 0.13 s/mol.
4053 Processing CHEMBL3818918 in molecule.smi (3709/4695). Average speed: 0.13 s/mol.
4054 Processing CHEMBL3818374 in molecule.smi (3711/4695). Average speed: 0.13 s/mol.
4055 Processing CHEMBL524100 in molecule.smi (3712/4695). Average speed: 0.13 s/mol.
4056 Processing CHEMBL489354 in molecule.smi (3713/4695). Average speed: 0.13 s/mol.
4057 Processing CHEMBL1254269 in molecule.smi (3714/4695). Average speed: 0.13 s/mol.
4058 Processing CHEMBL3819036 in molecule.smi (3715/4695). Average speed: 0.13 s/mol.
4059 Processing CHEMBL535 in molecule.smi (3716/4695). Average speed: 0.13 s/mol.
4060 Processing CHEMBL477772 in molecule.smi (3717/4695). Average speed: 0.13 s/mol.
4061 Processing CHEMBL3818089 in molecule.smi (3718/4695). Average speed: 0.13 s/mol.
4062 Processing CHEMBL3818086 in molecule.smi (3719/4695). Average speed: 0.13 s/mol.
4063 Processing CHEMBL3819231 in molecule.smi (3720/4695). Average speed: 0.13 s/mol.

4133 Processing CHEMBL3892044 in molecule.smi (3790/4695). Average speed: 0.13 s/mol.
4134 Processing CHEMBL3916769 in molecule.smi (3791/4695). Average speed: 0.13 s/mol.
4135 Processing CHEMBL3905695 in molecule.smi (3792/4695). Average speed: 0.13 s/mol.
4136 Processing CHEMBL3931599 in molecule.smi (3793/4695). Average speed: 0.13 s/mol.
4137 Processing CHEMBL3892118 in molecule.smi (3794/4695). Average speed: 0.13 s/mol.
4138 Processing CHEMBL3961103 in molecule.smi (3795/4695). Average speed: 0.13 s/mol.
4139 Processing CHEMBL3901082 in molecule.smi (3796/4695). Average speed: 0.13 s/mol.
4140 Processing CHEMBL3972214 in molecule.smi (3797/4695). Average speed: 0.13 s/mol.
4141 Processing CHEMBL3910142 in molecule.smi (3798/4695). Average speed: 0.13 s/mol.
4142 Processing CHEMBL8706 in molecule.smi (3799/4695). Average speed: 0.13 s/mol.
4143 Processing CHEMBL972 in molecule.smi (3800/4695). Average speed: 0.13 s/mol.
4144 Processing CHEMBL3291019 in molecule.smi (3801/4695). Average speed: 0.13 s/mol.
4145 Processing CHEMBL3960962 in molecule.smi (3802/4695). Average speed: 0.13 s/mol.
4146 Processing CHEMBL1903032 in molecule.smi (3803/4695). Average speed: 0.13 s/mol.
4147 Processing CHEMBL3931517 in molecule.smi (3804/4695). Average speed: 0.13 s/mol.
4148 Processing CHEMBL3939698 in molecule.smi (3806/4695). Average speed: 0.13 s/mol.
4149 Processing CHEMBL3969241 in molecule.smi (3805/4695). Average speed: 0.13 s/mol.
4150 Processing CHEMBL1485276 in molecule.smi (3807/4695). Average speed: 0.13 s/mol.
4151 Processing CHEMBL577016 in molecule.smi (3808/4695). Average speed: 0.13 s/mol.
4152 Processing CHEMBL3926757 in molecule.smi (3809/4695). Average speed: 0.13 s/mol.
4153 Processing CHEMBL3965046 in molecule.smi (3810/4695). Average speed: 0.13 s/mol.
4154 Processing CHEMBL1459580 in molecule.smi (3811/4695). Average speed: 0.13 s/mol.
4155 Processing CHEMBL3957099 in molecule.smi (3812/4695). Average speed: 0.13 s/mol.
4156 Processing CHEMBL3950130 in molecule.smi (3813/4695). Average speed: 0.13 s/mol.
4157 Processing CHEMBL611941 in molecule.smi (3814/4695). Average speed: 0.13 s/mol.
4158 Processing CHEMBL3921061 in molecule.smi (3815/4695). Average speed: 0.13 s/mol.
4159 Processing CHEMBL3948367 in molecule.smi (3816/4695). Average speed: 0.13 s/mol.
4160 Processing CHEMBL353468 in molecule.smi (3817/4695). Average speed: 0.13 s/mol.
4161 Processing CHEMBL170946 in molecule.smi (3818/4695). Average speed: 0.13 s/mol.
4162 Processing CHEMBL354848 in molecule.smi (3819/4695). Average speed: 0.13 s/mol.
4163 Processing CHEMBL3943450 in molecule.smi (3820/4695). Average speed: 0.13 s/mol.
4164 Processing CHEMBL3927363 in molecule.smi (3821/4695). Average speed: 0.13 s/mol.
4165 Processing CHEMBL3933395 in molecule.smi (3823/4695). Average speed: 0.13 s/mol.
4166 Processing CHEMBL3985059 in molecule.smi (3822/4695). Average speed: 0.13 s/mol.
4167 Processing CHEMBL3960861 in molecule.smi (3824/4695). Average speed: 0.13 s/mol.
4168 Processing CHEMBL3926911 in molecule.smi (3825/4695). Average speed: 0.13 s/mol.
4169 Processing CHEMBL3890758 in molecule.smi (3826/4695). Average speed: 0.13 s/mol.
4170 Processing CHEMBL3892502 in molecule.smi (3828/4695). Average speed: 0.13 s/mol.
4171 Processing CHEMBL3961494 in molecule.smi (3827/4695). Average speed: 0.13 s/mol.
4172 Processing CHEMBL145361 in molecule.smi (3829/4695). Average speed: 0.13 s/mol.
4173 Processing CHEMBL435071 in molecule.smi (3830/4695). Average speed: 0.13 s/mol.
4174 Processing CHEMBL3910513 in molecule.smi (3832/4695). Average speed: 0.13 s/mol.
4175 Processing CHEMBL171048 in molecule.smi (3831/4695). Average speed: 0.13 s/mol.
4176 Processing CHEMBL3900401 in molecule.smi (3835/4695). Average speed: 0.13 s/mol.
4177 Processing CHEMBL3891369 in molecule.smi (3833/4695). Average speed: 0.13 s/mol.
4178 Processing CHEMBL3919441 in molecule.smi (3834/4695). Average speed: 0.13 s/mol.
4179 Processing CHEMBL3928343 in molecule.smi (3836/4695). Average speed: 0.13 s/mol.
4180 Processing CHEMBL3944652 in molecule.smi (3837/4695). Average speed: 0.13 s/mol.
4181 Processing CHEMBL3973337 in molecule.smi (3838/4695). Average speed: 0.13 s/mol.
4182 Processing CHEMBL3889713 in molecule.smi (3839/4695). Average speed: 0.13 s/mol.
4183 Processing CHEMBL3889625 in molecule.smi (3840/4695). Average speed: 0.13 s/mol.
4184 Processing CHEMBL3950063 in molecule.smi (3842/4695). Average speed: 0.13 s/mol.
4185 Processing CHEMBL3934564 in molecule.smi (3841/4695). Average speed: 0.13 s/mol.
4186 Processing CHEMBL3984034 in molecule.smi (3843/4695). Average speed: 0.13 s/mol.
4187 Processing CHEMBL3955393 in molecule.smi (3844/4695). Average speed: 0.13 s/mol.
4188 Processing CHEMBL3976003 in molecule.smi (3845/4695). Average speed: 0.13 s/mol.
4189 Processing CHEMBL3928840 in molecule.smi (3846/4695). Average speed: 0.13 s/mol.
4190 Processing CHEMBL3983017 in molecule.smi (3847/4695). Average speed: 0.13 s/mol.
4191 Processing CHEMBL3901794 in molecule.smi (3848/4695). Average speed: 0.13 s/mol.
4192 Processing CHEMBL3972865 in molecule.smi (3849/4695). Average speed: 0.13 s/mol.
4193 Processing CHEMBL3910830 in molecule.smi (3850/4695). Average speed: 0.13 s/mol.
4194 Processing CHEMBL3945423 in molecule.smi (3851/4695). Average speed: 0.13 s/mol.
4195 Processing CHEMBL3930722 in molecule.smi (3852/4695). Average speed: 0.13 s/mol.
4196 Processing CHEMBL3958208 in molecule.smi (3853/4695). Average speed: 0.13 s/mol.
4197 Processing CHEMBL3921785 in molecule.smi (3854/4695). Average speed: 0.13 s/mol.
4198 Processing CHEMBL3948489 in molecule.smi (3855/4695). Average speed: 0.13 s/mol.
4199 Processing CHEMBL3884988 in molecule.smi (3856/4695). Average speed: 0.13 s/mol.
4200 Processing CHEMBL3884618 in molecule.smi (3857/4695). Average speed: 0.13 s/mol.
4201 Processing CHEMBL3884858 in molecule.smi (3858/4695). Average speed: 0.13 s/mol.

4202	Processing	CHEMBL3885186	in	molecule.smi	(3859/4695).	Average	speed:	0.13	s/mol.
4203	Processing	CHEMBL3884690	in	molecule.smi	(3860/4695).	Average	speed:	0.13	s/mol.
4204	Processing	CHEMBL3883432	in	molecule.smi	(3861/4695).	Average	speed:	0.13	s/mol.
4205	Processing	CHEMBL3971112	in	molecule.smi	(3862/4695).	Average	speed:	0.13	s/mol.
4206	Processing	CHEMBL3919289	in	molecule.smi	(3863/4695).	Average	speed:	0.13	s/mol.
4207	Processing	CHEMBL3922423	in	molecule.smi	(3864/4695).	Average	speed:	0.13	s/mol.
4208	Processing	CHEMBL3304357	in	molecule.smi	(3865/4695).	Average	speed:	0.13	s/mol.
4209	Processing	CHEMBL3304306	in	molecule.smi	(3866/4695).	Average	speed:	0.13	s/mol.
4210	Processing	CHEMBL4109726	in	molecule.smi	(3868/4695).	Average	speed:	0.13	s/mol.
4211	Processing	CHEMBL4113560	in	molecule.smi	(3867/4695).	Average	speed:	0.13	s/mol.
4212	Processing	CHEMBL3303094	in	molecule.smi	(3869/4695).	Average	speed:	0.13	s/mol.
4213	Processing	CHEMBL3304241	in	molecule.smi	(3870/4695).	Average	speed:	0.13	s/mol.
4214	Processing	CHEMBL4112162	in	molecule.smi	(3872/4695).	Average	speed:	0.13	s/mol.
4215	Processing	CHEMBL3304178	in	molecule.smi	(3871/4695).	Average	speed:	0.13	s/mol.
4216	Processing	CHEMBL3892148	in	molecule.smi	(3873/4695).	Average	speed:	0.13	s/mol.
4217	Processing	CHEMBL3937964	in	molecule.smi	(3874/4695).	Average	speed:	0.13	s/mol.
4218	Processing	CHEMBL3910025	in	molecule.smi	(3875/4695).	Average	speed:	0.13	s/mol.
4219	Processing	CHEMBL3952144	in	molecule.smi	(3876/4695).	Average	speed:	0.13	s/mol.
4220	Processing	CHEMBL3900968	in	molecule.smi	(3877/4695).	Average	speed:	0.13	s/mol.
4221	Processing	CHEMBL3947803	in	molecule.smi	(3878/4695).	Average	speed:	0.13	s/mol.
4222	Processing	CHEMBL3985136	in	molecule.smi	(3879/4695).	Average	speed:	0.13	s/mol.
4223	Processing	CHEMBL3959939	in	molecule.smi	(3880/4695).	Average	speed:	0.13	s/mol.
4224	Processing	CHEMBL3960964	in	molecule.smi	(3881/4695).	Average	speed:	0.13	s/mol.
4225	Processing	CHEMBL3933508	in	molecule.smi	(3882/4695).	Average	speed:	0.13	s/mol.
4226	Processing	CHEMBL3985662	in	molecule.smi	(3883/4695).	Average	speed:	0.13	s/mol.
4227	Processing	CHEMBL3939015	in	molecule.smi	(3884/4695).	Average	speed:	0.13	s/mol.
4228	Processing	CHEMBL3965431	in	molecule.smi	(3885/4695).	Average	speed:	0.13	s/mol.
4229	Processing	CHEMBL3981946	in	molecule.smi	(3886/4695).	Average	speed:	0.13	s/mol.
4230	Processing	CHEMBL3983878	in	molecule.smi	(3887/4695).	Average	speed:	0.13	s/mol.
4231	Processing	CHEMBL3928459	in	molecule.smi	(3888/4695).	Average	speed:	0.13	s/mol.
4232	Processing	CHEMBL3972317	in	molecule.smi	(3889/4695).	Average	speed:	0.13	s/mol.
4233	Processing	CHEMBL3949770	in	molecule.smi	(3890/4695).	Average	speed:	0.13	s/mol.
4234	Processing	CHEMBL3941497	in	molecule.smi	(3891/4695).	Average	speed:	0.13	s/mol.
4235	Processing	CHEMBL3922471	in	molecule.smi	(3892/4695).	Average	speed:	0.13	s/mol.
4236	Processing	CHEMBL3937974	in	molecule.smi	(3893/4695).	Average	speed:	0.13	s/mol.
4237	Processing	CHEMBL3910033	in	molecule.smi	(3894/4695).	Average	speed:	0.13	s/mol.
4238	Processing	CHEMBL3900977	in	molecule.smi	(3895/4695).	Average	speed:	0.13	s/mol.
4239	Processing	CHEMBL3895528	in	molecule.smi	(3896/4695).	Average	speed:	0.13	s/mol.
4240	Processing	CHEMBL3891315	in	molecule.smi	(3897/4695).	Average	speed:	0.13	s/mol.
4241	Processing	CHEMBL3986650	in	molecule.smi	(3898/4695).	Average	speed:	0.13	s/mol.
4242	Processing	CHEMBL3944088	in	molecule.smi	(3899/4695).	Average	speed:	0.13	s/mol.
4243	Processing	CHEMBL3938676	in	molecule.smi	(3901/4695).	Average	speed:	0.13	s/mol.
4244	Processing	CHEMBL3919972	in	molecule.smi	(3900/4695).	Average	speed:	0.13	s/mol.
4245	Processing	CHEMBL3968230	in	molecule.smi	(3902/4695).	Average	speed:	0.13	s/mol.
4246	Processing	CHEMBL3896153	in	molecule.smi	(3903/4695).	Average	speed:	0.13	s/mol.
4247	Processing	CHEMBL3920662	in	molecule.smi	(3904/4695).	Average	speed:	0.13	s/mol.
4248	Processing	CHEMBL3981703	in	molecule.smi	(3905/4695).	Average	speed:	0.13	s/mol.
4249	Processing	CHEMBL3911730	in	molecule.smi	(3906/4695).	Average	speed:	0.13	s/mol.
4250	Processing	CHEMBL4088116	in	molecule.smi	(3907/4695).	Average	speed:	0.13	s/mol.
4251	Processing	CHEMBL4093408	in	molecule.smi	(3908/4695).	Average	speed:	0.13	s/mol.
4252	Processing	CHEMBL4065799	in	molecule.smi	(3909/4695).	Average	speed:	0.13	s/mol.
4253	Processing	CHEMBL4103604	in	molecule.smi	(3911/4695).	Average	speed:	0.13	s/mol.
4254	Processing	CHEMBL4085671	in	molecule.smi	(3910/4695).	Average	speed:	0.13	s/mol.
4255	Processing	CHEMBL4063045	in	molecule.smi	(3912/4695).	Average	speed:	0.13	s/mol.
4256	Processing	CHEMBL4086323	in	molecule.smi	(3914/4695).	Average	speed:	0.13	s/mol.
4257	Processing	CHEMBL4084714	in	molecule.smi	(3913/4695).	Average	speed:	0.13	s/mol.
4258	Processing	CHEMBL4064846	in	molecule.smi	(3915/4695).	Average	speed:	0.13	s/mol.
4259	Processing	CHEMBL4078463	in	molecule.smi	(3916/4695).	Average	speed:	0.13	s/mol.
4260	Processing	CHEMBL4102718	in	molecule.smi	(3917/4695).	Average	speed:	0.13	s/mol.
4261	Processing	CHEMBL4067562	in	molecule.smi	(3918/4695).	Average	speed:	0.13	s/mol.
4262	Processing	CHEMBL4094981	in	molecule.smi	(3919/4695).	Average	speed:	0.13	s/mol.
4263	Processing	CHEMBL4105158	in	molecule.smi	(3920/4695).	Average	speed:	0.13	s/mol.
4264	Processing	CHEMBL4087300	in	molecule.smi	(3921/4695).	Average	speed:	0.13	s/mol.
4265	Processing	CHEMBL4072405	in	molecule.smi	(3922/4695).	Average	speed:	0.13	s/mol.
4266	Processing	CHEMBL4099340	in	molecule.smi	(3923/4695).	Average	speed:	0.13	s/mol.
4267	Processing	CHEMBL4087978	in	molecule.smi	(3924/4695).	Average	speed:	0.13	s/mol.
4268	Processing	CHEMBL4059684	in	molecule.smi	(3925/4695).	Average	speed:	0.13	s/mol.
4269	Processing	CHEMBL4095695	in	molecule.smi	(3926/4695).	Average	speed:	0.13	s/mol.
4270	Processing	CHEMBL4068340	in	molecule.smi	(3927/4695).	Average	speed:	0.13	s/mol.

4271	Processing	CHEMBL4090413	in molecule.smi	(3929/4695)	Average speed: 0.13 s/mol.
4272	Processing	CHEMBL4069385	in molecule.smi	(3928/4695)	Average speed: 0.13 s/mol.
4273	Processing	CHEMBL4080105	in molecule.smi	(3930/4695)	Average speed: 0.13 s/mol.
4274	Processing	CHEMBL4098132	in molecule.smi	(3931/4695)	Average speed: 0.13 s/mol.
4275	Processing	CHEMBL4074258	in molecule.smi	(3932/4695)	Average speed: 0.13 s/mol.
4276	Processing	CHEMBL4094761	in molecule.smi	(3933/4695)	Average speed: 0.13 s/mol.
4277	Processing	CHEMBL4075021	in molecule.smi	(3934/4695)	Average speed: 0.13 s/mol.
4278	Processing	CHEMBL4101703	in molecule.smi	(3935/4695)	Average speed: 0.13 s/mol.
4279	Processing	CHEMBL4085283	in molecule.smi	(3936/4695)	Average speed: 0.13 s/mol.
4280	Processing	CHEMBL4063663	in molecule.smi	(3937/4695)	Average speed: 0.13 s/mol.
4281	Processing	CHEMBL4093019	in molecule.smi	(3938/4695)	Average speed: 0.13 s/mol.
4282	Processing	CHEMBL4072258	in molecule.smi	(3939/4695)	Average speed: 0.13 s/mol.
4283	Processing	CHEMBL4100736	in molecule.smi	(3940/4695)	Average speed: 0.13 s/mol.
4284	Processing	CHEMBL4082739	in molecule.smi	(3941/4695)	Average speed: 0.13 s/mol.
4285	Processing	CHEMBL4062593	in molecule.smi	(3942/4695)	Average speed: 0.13 s/mol.
4286	Processing	CHEMBL4090559	in molecule.smi	(3943/4695)	Average speed: 0.13 s/mol.
4287	Processing	CHEMBL4103664	in molecule.smi	(3944/4695)	Average speed: 0.13 s/mol.
4288	Processing	CHEMBL4085738	in molecule.smi	(3945/4695)	Average speed: 0.13 s/mol.
4289	Processing	CHEMBL4095908	in molecule.smi	(3946/4695)	Average speed: 0.13 s/mol.
4290	Processing	CHEMBL4104551	in molecule.smi	(3947/4695)	Average speed: 0.13 s/mol.
4291	Processing	CHEMBL4067497	in molecule.smi	(3948/4695)	Average speed: 0.13 s/mol.
4292	Processing	CHEMBL4089082	in molecule.smi	(3949/4695)	Average speed: 0.13 s/mol.
4293	Processing	CHEMBL4075571	in molecule.smi	(3951/4695)	Average speed: 0.13 s/mol.
4294	Processing	CHEMBL4090583	in molecule.smi	(3950/4695)	Average speed: 0.13 s/mol.
4295	Processing	CHEMBL4094805	in molecule.smi	(3952/4695)	Average speed: 0.13 s/mol.
4296	Processing	CHEMBL4100760	in molecule.smi	(3953/4695)	Average speed: 0.13 s/mol.
4297	Processing	CHEMBL4059887	in molecule.smi	(3954/4695)	Average speed: 0.13 s/mol.
4298	Processing	CHEMBL4081805	in molecule.smi	(3955/4695)	Average speed: 0.13 s/mol.
4299	Processing	CHEMBL4098196	in molecule.smi	(3956/4695)	Average speed: 0.13 s/mol.
4300	Processing	CHEMBL4102562	in molecule.smi	(3957/4695)	Average speed: 0.13 s/mol.
4301	Processing	CHEMBL4072914	in molecule.smi	(3958/4695)	Average speed: 0.13 s/mol.
4302	Processing	CHEMBL4069184	in molecule.smi	(3959/4695)	Average speed: 0.13 s/mol.
4303	Processing	CHEMBL4060687	in molecule.smi	(3960/4695)	Average speed: 0.13 s/mol.
4304	Processing	CHEMBL4081013	in molecule.smi	(3961/4695)	Average speed: 0.13 s/mol.
4305	Processing	CHEMBL4099046	in molecule.smi	(3962/4695)	Average speed: 0.13 s/mol.
4306	Processing	CHEMBL4091317	in molecule.smi	(3964/4695)	Average speed: 0.13 s/mol.
4307	Processing	CHEMBL4070380	in molecule.smi	(3963/4695)	Average speed: 0.13 s/mol.
4308	Processing	CHEMBL4061746	in molecule.smi	(3965/4695)	Average speed: 0.13 s/mol.
4309	Processing	CHEMBL4083524	in molecule.smi	(3966/4695)	Average speed: 0.13 s/mol.
4310	Processing	CHEMBL4097374	in molecule.smi	(3967/4695)	Average speed: 0.13 s/mol.
4311	Processing	CHEMBL4079345	in molecule.smi	(3968/4695)	Average speed: 0.13 s/mol.
4312	Processing	CHEMBL4105088	in molecule.smi	(3969/4695)	Average speed: 0.13 s/mol.
4313	Processing	CHEMBL3262251	in molecule.smi	(3970/4695)	Average speed: 0.13 s/mol.
4314	Processing	CHEMBL4067481	in molecule.smi	(3971/4695)	Average speed: 0.13 s/mol.
4315	Processing	CHEMBL4094911	in molecule.smi	(3972/4695)	Average speed: 0.13 s/mol.
4316	Processing	CHEMBL4078382	in molecule.smi	(3973/4695)	Average speed: 0.13 s/mol.
4317	Processing	CHEMBL4102655	in molecule.smi	(3974/4695)	Average speed: 0.13 s/mol.
4318	Processing	CHEMBL4086248	in molecule.smi	(3975/4695)	Average speed: 0.13 s/mol.
4319	Processing	CHEMBL4064773	in molecule.smi	(3976/4695)	Average speed: 0.13 s/mol.
4320	Processing	CHEMBL4061837	in molecule.smi	(3977/4695)	Average speed: 0.13 s/mol.
4321	Processing	CHEMBL4070462	in molecule.smi	(3979/4695)	Average speed: 0.13 s/mol.
4322	Processing	CHEMBL4083601	in molecule.smi	(3978/4695)	Average speed: 0.13 s/mol.
4323	Processing	CHEMBL4100046	in molecule.smi	(3981/4695)	Average speed: 0.13 s/mol.
4324	Processing	CHEMBL4091385	in molecule.smi	(3980/4695)	Average speed: 0.13 s/mol.
4325	Processing	CHEMBL4096673	in molecule.smi	(3983/4695)	Average speed: 0.13 s/mol.
4326	Processing	CHEMBL4073193	in molecule.smi	(3982/4695)	Average speed: 0.13 s/mol.
4327	Processing	CHEMBL4060016	in molecule.smi	(3985/4695)	Average speed: 0.13 s/mol.
4328	Processing	CHEMBL4069444	in molecule.smi	(3984/4695)	Average speed: 0.13 s/mol.
4329	Processing	CHEMBL4085114	in molecule.smi	(3986/4695)	Average speed: 0.13 s/mol.
4330	Processing	CHEMBL4098421	in molecule.smi	(3987/4695)	Average speed: 0.13 s/mol.
4331	Processing	CHEMBL4077088	in molecule.smi	(3988/4695)	Average speed: 0.13 s/mol.
4332	Processing	CHEMBL4099790	in molecule.smi	(3989/4695)	Average speed: 0.13 s/mol.
4333	Processing	CHEMBL1626455	in molecule.smi	(3990/4695)	Average speed: 0.13 s/mol.
4334	Processing	CHEMBL4095445	in molecule.smi	(3991/4695)	Average speed: 0.13 s/mol.
4335	Processing	CHEMBL2337271	in molecule.smi	(3992/4695)	Average speed: 0.13 s/mol.
4336	Processing	CHEMBL215645	in molecule.smi	(3993/4695)	Average speed: 0.13 s/mol.
4337	Processing	CHEMBL4081795	in molecule.smi	(3995/4695)	Average speed: 0.13 s/mol.
4338	Processing	CHEMBL4060617	in molecule.smi	(3994/4695)	Average speed: 0.13 s/mol.
4339	Processing	CHEMBL4066309	in molecule.smi	(3996/4695)	Average speed: 0.13 s/mol.

4340 Processing CHEMBL4093419 in molecule.smi (3997/4695). Average speed: 0.13 s/mol.
4341 Processing CHEMBL4083174 in molecule.smi (3998/4695). Average speed: 0.13 s/mol.
4342 Processing CHEMBL521589 in molecule.smi (3999/4695). Average speed: 0.13 s/mol.
4343 Processing CHEMBL4096024 in molecule.smi (4000/4695). Average speed: 0.13 s/mol.
4344 Processing CHEMBL4098455 in molecule.smi (4001/4695). Average speed: 0.13 s/mol.
4345 Processing CHEMBL4099598 in molecule.smi (4002/4695). Average speed: 0.13 s/mol.
4346 Processing CHEMBL4083875 in molecule.smi (4004/4695). Average speed: 0.13 s/mol.
4347 Processing CHEMBL4062146 in molecule.smi (4003/4695). Average speed: 0.13 s/mol.
4348 Processing CHEMBL4070769 in molecule.smi (4005/4695). Average speed: 0.13 s/mol.
4349 Processing CHEMBL4091651 in molecule.smi (4006/4695). Average speed: 0.13 s/mol.
4350 Processing CHEMBL4092602 in molecule.smi (4007/4695). Average speed: 0.13 s/mol.
4351 Processing CHEMBL4064904 in molecule.smi (4008/4695). Average speed: 0.13 s/mol.
4352 Processing CHEMBL4100338 in molecule.smi (4009/4695). Average speed: 0.13 s/mol.
4353 Processing CHEMBL4074566 in molecule.smi (4011/4695). Average speed: 0.13 s/mol.
4354 Processing CHEMBL4073501 in molecule.smi (4010/4695). Average speed: 0.13 s/mol.
4355 Processing CHEMBL4095032 in molecule.smi (4012/4695). Average speed: 0.13 s/mol.
4356 Processing CHEMBL4060800 in molecule.smi (4013/4695). Average speed: 0.13 s/mol.
4357 Processing CHEMBL4085222 in molecule.smi (4014/4695). Average speed: 0.13 s/mol.
4358 Processing CHEMBL4092048 in molecule.smi (4015/4695). Average speed: 0.13 s/mol.
4359 Processing CHEMBL4061527 in molecule.smi (4016/4695). Average speed: 0.13 s/mol.
4360 Processing CHEMBL4081776 in molecule.smi (4017/4695). Average speed: 0.13 s/mol.
4361 Processing CHEMBL4099794 in molecule.smi (4018/4695). Average speed: 0.13 s/mol.
4362 Processing CHEMBL4105085 in molecule.smi (4019/4695). Average speed: 0.13 s/mol.
4363 Processing CHEMBL4083445 in molecule.smi (4020/4695). Average speed: 0.13 s/mol.
4364 Processing CHEMBL4093567 in molecule.smi (4021/4695). Average speed: 0.13 s/mol.
4365 Processing CHEMBL4072865 in molecule.smi (4022/4695). Average speed: 0.13 s/mol.
4366 Processing CHEMBL4101303 in molecule.smi (4023/4695). Average speed: 0.13 s/mol.
4367 Processing CHEMBL4076930 in molecule.smi (4024/4695). Average speed: 0.13 s/mol.
4368 Processing CHEMBL4095535 in molecule.smi (4025/4695). Average speed: 0.13 s/mol.
4369 Processing CHEMBL4068149 in molecule.smi (4026/4695). Average speed: 0.13 s/mol.
4370 Processing CHEMBL4092123 in molecule.smi (4027/4695). Average speed: 0.13 s/mol.
4371 Processing CHEMBL4064413 in molecule.smi (4028/4695). Average speed: 0.13 s/mol.
4372 Processing CHEMBL4072999 in molecule.smi (4030/4695). Average speed: 0.13 s/mol.
4373 Processing CHEMBL4099873 in molecule.smi (4029/4695). Average speed: 0.13 s/mol.
4374 Processing CHEMBL4074062 in molecule.smi (4031/4695). Average speed: 0.13 s/mol.
4375 Processing CHEMBL4094591 in molecule.smi (4032/4695). Average speed: 0.13 s/mol.
4376 Processing CHEMBL4102333 in molecule.smi (4034/4695). Average speed: 0.13 s/mol.
4377 Processing CHEMBL4084371 in molecule.smi (4033/4695). Average speed: 0.13 s/mol.
4378 Processing CHEMBL4066548 in molecule.smi (4035/4695). Average speed: 0.13 s/mol.
4379 Processing CHEMBL4094081 in molecule.smi (4036/4695). Average speed: 0.13 s/mol.
4380 Processing CHEMBL4081915 in molecule.smi (4037/4695). Average speed: 0.13 s/mol.
4381 Processing CHEMBL4060011 in molecule.smi (4038/4695). Average speed: 0.13 s/mol.
4382 Processing CHEMBL4071377 in molecule.smi (4039/4695). Average speed: 0.13 s/mol.
4383 Processing CHEMBL4098418 in molecule.smi (4040/4695). Average speed: 0.13 s/mol.
4384 Processing CHEMBL4083306 in molecule.smi (4041/4695). Average speed: 0.13 s/mol.
4385 Processing CHEMBL4077952 in molecule.smi (4042/4695). Average speed: 0.13 s/mol.
4386 Processing CHEMBL4076034 in molecule.smi (4043/4695). Average speed: 0.13 s/mol.
4387 Processing CHEMBL4070182 in molecule.smi (4044/4695). Average speed: 0.13 s/mol.
4388 Processing CHEMBL4075061 in molecule.smi (4046/4695). Average speed: 0.13 s/mol.
4389 Processing CHEMBL4091851 in molecule.smi (4045/4695). Average speed: 0.13 s/mol.
4390 Processing CHEMBL4066365 in molecule.smi (4047/4695). Average speed: 0.13 s/mol.
4391 Processing CHEMBL4093928 in molecule.smi (4048/4695). Average speed: 0.13 s/mol.
4392 Processing CHEMBL4097266 in molecule.smi (4049/4695). Average speed: 0.13 s/mol.
4393 Processing CHEMBL4072457 in molecule.smi (4050/4695). Average speed: 0.13 s/mol.
4394 Processing CHEMBL23838 in molecule.smi (4051/4695). Average speed: 0.13 s/mol.
4395 Processing CHEMBL4060832 in molecule.smi (4052/4695). Average speed: 0.13 s/mol.
4396 Processing CHEMBL4089033 in molecule.smi (4053/4695). Average speed: 0.13 s/mol.
4397 Processing CHEMBL4088091 in molecule.smi (4054/4695). Average speed: 0.13 s/mol.
4398 Processing CHEMBL4066805 in molecule.smi (4055/4695). Average speed: 0.13 s/mol.
4399 Processing CHEMBL4080216 in molecule.smi (4056/4695). Average speed: 0.13 s/mol.
4400 Processing CHEMBL4072825 in molecule.smi (4058/4695). Average speed: 0.13 s/mol.
4401 Processing CHEMBL4104459 in molecule.smi (4057/4695). Average speed: 0.13 s/mol.
4402 Processing CHEMBL4093532 in molecule.smi (4059/4695). Average speed: 0.13 s/mol.
4403 Processing CHEMBL4069096 in molecule.smi (4060/4695). Average speed: 0.13 s/mol.
4404 Processing CHEMBL4090159 in molecule.smi (4061/4695). Average speed: 0.13 s/mol.
4405 Processing CHEMBL4079853 in molecule.smi (4062/4695). Average speed: 0.13 s/mol.
4406 Processing CHEMBL4097877 in molecule.smi (4063/4695). Average speed: 0.13 s/mol.
4407 Processing CHEMBL4098808 in molecule.smi (4064/4695). Average speed: 0.13 s/mol.
4408 Processing CHEMBL4071803 in molecule.smi (4065/4695). Average speed: 0.13 s/mol.

4409 Processing CHEMBL4085482 in molecule.smi (4066/4695). Average speed: 0.13 s/mol.
4410 Processing CHEMBL4082785 in molecule.smi (4067/4695). Average speed: 0.13 s/mol.
4411 Processing CHEMBL4072478 in molecule.smi (4068/4695). Average speed: 0.13 s/mol.
4412 Processing CHEMBL4101886 in molecule.smi (4069/4695). Average speed: 0.13 s/mol.
4413 Processing CHEMBL4068410 in molecule.smi (4070/4695). Average speed: 0.13 s/mol.
4414 Processing CHEMBL4095755 in molecule.smi (4071/4695). Average speed: 0.13 s/mol.
4415 Processing CHEMBL4090842 in molecule.smi (4072/4695). Average speed: 0.13 s/mol.
4416 Processing CHEMBL4069847 in molecule.smi (4073/4695). Average speed: 0.13 s/mol.
4417 Processing CHEMBL4091748 in molecule.smi (4075/4695). Average speed: 0.13 s/mol.
4418 Processing CHEMBL4063984 in molecule.smi (4074/4695). Average speed: 0.13 s/mol.
4419 Processing CHEMBL4072579 in molecule.smi (4076/4695). Average speed: 0.13 s/mol.
4420 Processing CHEMBL4099486 in molecule.smi (4077/4695). Average speed: 0.13 s/mol.
4421 Processing CHEMBL4068829 in molecule.smi (4078/4695). Average speed: 0.13 s/mol.
4422 Processing CHEMBL4096126 in molecule.smi (4079/4695). Average speed: 0.13 s/mol.
4423 Processing CHEMBL4059560 in molecule.smi (4080/4695). Average speed: 0.13 s/mol.
4424 Processing CHEMBL4081509 in molecule.smi (4081/4695). Average speed: 0.13 s/mol.
4425 Processing CHEMBL4098703 in molecule.smi (4082/4695). Average speed: 0.13 s/mol.
4426 Processing CHEMBL4076580 in molecule.smi (4083/4695). Average speed: 0.13 s/mol.
4427 Processing CHEMBL4095035 in molecule.smi (4084/4695). Average speed: 0.13 s/mol.
4428 Processing CHEMBL4073287 in molecule.smi (4085/4695). Average speed: 0.13 s/mol.
4429 Processing CHEMBL4099391 in molecule.smi (4086/4695). Average speed: 0.13 s/mol.
4430 Processing CHEMBL4084842 in molecule.smi (4087/4695). Average speed: 0.13 s/mol.
4431 Processing CHEMBL4076986 in molecule.smi (4088/4695). Average speed: 0.13 s/mol.
4432 Processing CHEMBL4063583 in molecule.smi (4089/4695). Average speed: 0.13 s/mol.
4433 Processing CHEMBL4082048 in molecule.smi (4090/4695). Average speed: 0.13 s/mol.
4434 Processing CHEMBL4083039 in molecule.smi (4091/4695). Average speed: 0.13 s/mol.
4435 Processing CHEMBL4101018 in molecule.smi (4092/4695). Average speed: 0.13 s/mol.
4436 Processing CHEMBL4070471 in molecule.smi (4093/4695). Average speed: 0.13 s/mol.
4437 Processing CHEMBL1340607 in molecule.smi (4094/4695). Average speed: 0.13 s/mol.
4438 Processing CHEMBL1482486 in molecule.smi (4095/4695). Average speed: 0.13 s/mol.
4439 Processing CHEMBL4081932 in molecule.smi (4096/4695). Average speed: 0.13 s/mol.
4440 Processing CHEMBL4099934 in molecule.smi (4097/4695). Average speed: 0.13 s/mol.
4441 Processing CHEMBL4071394 in molecule.smi (4098/4695). Average speed: 0.13 s/mol.
4442 Processing CHEMBL4092186 in molecule.smi (4099/4695). Average speed: 0.13 s/mol.
4443 Processing CHEMBL1543212 in molecule.smi (4100/4695). Average speed: 0.13 s/mol.
4444 Processing CHEMBL1416246 in molecule.smi (4101/4695). Average speed: 0.13 s/mol.
4445 Processing CHEMBL4095547 in molecule.smi (4102/4695). Average speed: 0.13 s/mol.
4446 Processing CHEMBL4075136 in molecule.smi (4103/4695). Average speed: 0.13 s/mol.
4447 Processing CHEMBL1301463 in molecule.smi (4105/4695). Average speed: 0.13 s/mol.
4448 Processing CHEMBL4087841 in molecule.smi (4104/4695). Average speed: 0.13 s/mol.
4449 Processing CHEMBL4079963 in molecule.smi (4106/4695). Average speed: 0.13 s/mol.
4450 Processing CHEMBL179218 in molecule.smi (4109/4695). Average speed: 0.13 s/mol.
4451 Processing CHEMBL4092142 in molecule.smi (4108/4695). Average speed: 0.13 s/mol.
4452 Processing CHEMBL4104206 in molecule.smi (4107/4695). Average speed: 0.13 s/mol.
4453 Processing CHEMBL4064806 in molecule.smi (4110/4695). Average speed: 0.13 s/mol.
4454 Processing CHEMBL4100253 in molecule.smi (4111/4695). Average speed: 0.13 s/mol.
4455 Processing CHEMBL4073401 in molecule.smi (4112/4695). Average speed: 0.13 s/mol.
4456 Processing CHEMBL1311140 in molecule.smi (4113/4695). Average speed: 0.13 s/mol.
4457 Processing CHEMBL14577 in molecule.smi (4114/4695). Average speed: 0.13 s/mol.
4458 Processing CHEMBL4068713 in molecule.smi (4116/4695). Average speed: 0.13 s/mol.
4459 Processing CHEMBL451635 in molecule.smi (4115/4695). Average speed: 0.13 s/mol.
4460 Processing CHEMBL4088294 in molecule.smi (4117/4695). Average speed: 0.13 s/mol.
4461 Processing CHEMBL4060058 in molecule.smi (4118/4695). Average speed: 0.13 s/mol.
4462 Processing CHEMBL4080917 in molecule.smi (4119/4695). Average speed: 0.13 s/mol.
4463 Processing CHEMBL4104406 in molecule.smi (4120/4695). Average speed: 0.13 s/mol.
4464 Processing CHEMBL4062826 in molecule.smi (4121/4695). Average speed: 0.13 s/mol.
4465 Processing CHEMBL4073838 in molecule.smi (4123/4695). Average speed: 0.13 s/mol.
4466 Processing CHEMBL4100057 in molecule.smi (4122/4695). Average speed: 0.13 s/mol.
4467 Processing CHEMBL4100639 in molecule.smi (4124/4695). Average speed: 0.13 s/mol.
4468 Processing CHEMBL4065242 in molecule.smi (4125/4695). Average speed: 0.13 s/mol.
4469 Processing CHEMBL4092905 in molecule.smi (4126/4695). Average speed: 0.13 s/mol.
4470 Processing CHEMBL4091945 in molecule.smi (4127/4695). Average speed: 0.13 s/mol.
4471 Processing CHEMBL4076907 in molecule.smi (4128/4695). Average speed: 0.13 s/mol.
4472 Processing CHEMBL4084189 in molecule.smi (4129/4695). Average speed: 0.13 s/mol.
4473 Processing CHEMBL4062487 in molecule.smi (4130/4695). Average speed: 0.13 s/mol.
4474 Processing CHEMBL4061404 in molecule.smi (4131/4695). Average speed: 0.13 s/mol.
4475 Processing CHEMBL4102122 in molecule.smi (4133/4695). Average speed: 0.13 s/mol.
4476 Processing CHEMBL4089550 in molecule.smi (4132/4695). Average speed: 0.13 s/mol.
4477 Processing CHEMBL4077866 in molecule.smi (4134/4695). Average speed: 0.13 s/mol.

4478 Processing CHEMBL4064154 in molecule.smi (4135/4695). Average speed: 0.13 s/mol.
4479 Processing CHEMBL4085722 in molecule.smi (4136/4695). Average speed: 0.13 s/mol.
4480 Processing CHEMBL4086639 in molecule.smi (4137/4695). Average speed: 0.13 s/mol.
4481 Processing CHEMBL4104534 in molecule.smi (4138/4695). Average speed: 0.13 s/mol.
4482 Processing CHEMBL4094380 in molecule.smi (4139/4695). Average speed: 0.13 s/mol.
4483 Processing CHEMBL4066891 in molecule.smi (4140/4695). Average speed: 0.13 s/mol.
4484 Processing CHEMBL4091001 in molecule.smi (4141/4695). Average speed: 0.13 s/mol.
4485 Processing CHEMBL4063109 in molecule.smi (4142/4695). Average speed: 0.13 s/mol.
4486 Processing CHEMBL4064304 in molecule.smi (4143/4695). Average speed: 0.13 s/mol.
4487 Processing CHEMBL4080800 in molecule.smi (4144/4695). Average speed: 0.13 s/mol.
4488 Processing CHEMBL4094837 in molecule.smi (4145/4695). Average speed: 0.13 s/mol.
4489 Processing CHEMBL4090498 in molecule.smi (4146/4695). Average speed: 0.13 s/mol.
4490 Processing CHEMBL4069472 in molecule.smi (4147/4695). Average speed: 0.13 s/mol.
4491 Processing CHEMBL4104952 in molecule.smi (4148/4695). Average speed: 0.13 s/mol.
4492 Processing CHEMBL4080726 in molecule.smi (4149/4695). Average speed: 0.13 s/mol.
4493 Processing CHEMBL4097249 in molecule.smi (4150/4695). Average speed: 0.13 s/mol.
4494 Processing CHEMBL4070057 in molecule.smi (4151/4695). Average speed: 0.13 s/mol.
4495 Processing CHEMBL4078265 in molecule.smi (4152/4695). Average speed: 0.13 s/mol.
4496 Processing CHEMBL4096311 in molecule.smi (4153/4695). Average speed: 0.13 s/mol.
4497 Processing CHEMBL4067342 in molecule.smi (4154/4695). Average speed: 0.13 s/mol.
4498 Processing CHEMBL4071110 in molecule.smi (4156/4695). Average speed: 0.13 s/mol.
4499 Processing CHEMBL4088594 in molecule.smi (4155/4695). Average speed: 0.13 s/mol.
4500 Processing CHEMBL4091935 in molecule.smi (4157/4695). Average speed: 0.13 s/mol.
4501 Processing CHEMBL4070092 in molecule.smi (4158/4695). Average speed: 0.13 s/mol.
4502 Processing CHEMBL4065259 in molecule.smi (4160/4695). Average speed: 0.13 s/mol.
4503 Processing CHEMBL4077169 in molecule.smi (4159/4695). Average speed: 0.13 s/mol.
4504 Processing CHEMBL4075825 in molecule.smi (4161/4695). Average speed: 0.13 s/mol.
4505 Processing CHEMBL4075624 in molecule.smi (4162/4695). Average speed: 0.13 s/mol.
4506 Processing CHEMBL4088659 in molecule.smi (4163/4695). Average speed: 0.13 s/mol.
4507 Processing CHEMBL4063635 in molecule.smi (4165/4695). Average speed: 0.13 s/mol.
4508 Processing CHEMBL4074993 in molecule.smi (4164/4695). Average speed: 0.13 s/mol.
4509 Processing CHEMBL4083288 in molecule.smi (4166/4695). Average speed: 0.13 s/mol.
4510 Processing CHEMBL4066908 in molecule.smi (4167/4695). Average speed: 0.13 s/mol.
4511 Processing CHEMBL4075667 in molecule.smi (4168/4695). Average speed: 0.13 s/mol.
4512 Processing CHEMBL4091683 in molecule.smi (4169/4695). Average speed: 0.13 s/mol.
4513 Processing CHEMBL4069776 in molecule.smi (4170/4695). Average speed: 0.13 s/mol.
4514 Processing CHEMBL4096963 in molecule.smi (4171/4695). Average speed: 0.13 s/mol.
4515 Processing CHEMBL4089264 in molecule.smi (4172/4695). Average speed: 0.13 s/mol.
4516 Processing CHEMBL887 in molecule.smi (4173/4695). Average speed: 0.13 s/mol.
4517 Processing CHEMBL3425894 in molecule.smi (4175/4695). Average speed: 0.13 s/mol.
4518 Processing CHEMBL3425895 in molecule.smi (4174/4695). Average speed: 0.13 s/mol.
4519 Processing CHEMBL3425893 in molecule.smi (4176/4695). Average speed: 0.13 s/mol.
4520 Processing CHEMBL3425892 in molecule.smi (4177/4695). Average speed: 0.13 s/mol.
4521 Processing CHEMBL3425889 in molecule.smi (4178/4695). Average speed: 0.13 s/mol.
4522 Processing CHEMBL1303143 in molecule.smi (4179/4695). Average speed: 0.13 s/mol.
4523 Processing CHEMBL3425881 in molecule.smi (4180/4695). Average speed: 0.13 s/mol.
4524 Processing CHEMBL3425891 in molecule.smi (4181/4695). Average speed: 0.13 s/mol.
4525 Processing CHEMBL3425890 in molecule.smi (4182/4695). Average speed: 0.13 s/mol.
4526 Processing CHEMBL3425885 in molecule.smi (4183/4695). Average speed: 0.13 s/mol.
4527 Processing CHEMBL1242180 in molecule.smi (4184/4695). Average speed: 0.13 s/mol.
4528 Processing CHEMBL4097284 in molecule.smi (4186/4695). Average speed: 0.13 s/mol.
4529 Processing CHEMBL4061433 in molecule.smi (4185/4695). Average speed: 0.13 s/mol.
4530 Processing CHEMBL4070093 in molecule.smi (4187/4695). Average speed: 0.13 s/mol.
4531 Processing CHEMBL4093946 in molecule.smi (4188/4695). Average speed: 0.13 s/mol.
4532 Processing CHEMBL4066392 in molecule.smi (4189/4695). Average speed: 0.13 s/mol.
4533 Processing CHEMBL4104589 in molecule.smi (4191/4695). Average speed: 0.13 s/mol.
4534 Processing CHEMBL4080358 in molecule.smi (4190/4695). Average speed: 0.13 s/mol.
4535 Processing CHEMBL597863 in molecule.smi (4192/4695). Average speed: 0.13 s/mol.
4536 Processing CHEMBL4096862 in molecule.smi (4193/4695). Average speed: 0.13 s/mol.
4537 Processing CHEMBL4060972 in molecule.smi (4194/4695). Average speed: 0.13 s/mol.
4538 Processing CHEMBL4089155 in molecule.smi (4195/4695). Average speed: 0.13 s/mol.
4539 Processing CHEMBL4099308 in molecule.smi (4196/4695). Average speed: 0.13 s/mol.
4540 Processing CHEMBL4086152 in molecule.smi (4197/4695). Average speed: 0.13 s/mol.
4541 Processing CHEMBL4093514 in molecule.smi (4199/4695). Average speed: 0.13 s/mol.
4542 Processing CHEMBL4065910 in molecule.smi (4198/4695). Average speed: 0.13 s/mol.
4543 Processing CHEMBL4086383 in molecule.smi (4200/4695). Average speed: 0.13 s/mol.
4544 Processing CHEMBL4078528 in molecule.smi (4202/4695). Average speed: 0.13 s/mol.
4545 Processing CHEMBL4064920 in molecule.smi (4201/4695). Average speed: 0.13 s/mol.
4546 Processing CHEMBL4102810 in molecule.smi (4203/4695). Average speed: 0.13 s/mol.

4616 Processing CHEMBL4164525 in molecule.smi (4273/4695). Average speed: 0.13 s/mol.
4617 Processing CHEMBL4160912 in molecule.smi (4274/4695). Average speed: 0.13 s/mol.
4618 Processing CHEMBL4164315 in molecule.smi (4275/4695). Average speed: 0.13 s/mol.
4619 Processing CHEMBL4167757 in molecule.smi (4277/4695). Average speed: 0.13 s/mol.
4620 Processing CHEMBL4174963 in molecule.smi (4276/4695). Average speed: 0.13 s/mol.
4621 Processing CHEMBL4159837 in molecule.smi (4278/4695). Average speed: 0.13 s/mol.
4622 Processing CHEMBL4164387 in molecule.smi (4279/4695). Average speed: 0.13 s/mol.
4623 Processing CHEMBL4165897 in molecule.smi (4280/4695). Average speed: 0.13 s/mol.
4624 Processing CHEMBL4173815 in molecule.smi (4281/4695). Average speed: 0.13 s/mol.
4625 Processing CHEMBL4162452 in molecule.smi (4282/4695). Average speed: 0.13 s/mol.
4626 Processing CHEMBL4170372 in molecule.smi (4283/4695). Average speed: 0.13 s/mol.
4627 Processing CHEMBL4162043 in molecule.smi (4284/4695). Average speed: 0.13 s/mol.
4628 Processing CHEMBL4169326 in molecule.smi (4285/4695). Average speed: 0.13 s/mol.
4629 Processing CHEMBL4177164 in molecule.smi (4286/4695). Average speed: 0.13 s/mol.
4630 Processing CHEMBL4160856 in molecule.smi (4287/4695). Average speed: 0.13 s/mol.
4631 Processing CHEMBL4168790 in molecule.smi (4288/4695). Average speed: 0.13 s/mol.
4632 Processing CHEMBL469638 in molecule.smi (4290/4695). Average speed: 0.13 s/mol.
4633 Processing CHEMBL4167958 in molecule.smi (4289/4695). Average speed: 0.13 s/mol.
4634 Processing CHEMBL586091 in molecule.smi (4291/4695). Average speed: 0.13 s/mol.
4635 Processing CHEMBL1172893 in molecule.smi (4292/4695). Average speed: 0.13 s/mol.
4636 Processing CHEMBL4172271 in molecule.smi (4293/4695). Average speed: 0.13 s/mol.
4637 Processing CHEMBL4172720 in molecule.smi (4294/4695). Average speed: 0.13 s/mol.
4638 Processing CHEMBL4163781 in molecule.smi (4295/4695). Average speed: 0.12 s/mol.
4639 Processing CHEMBL4165299 in molecule.smi (4296/4695). Average speed: 0.12 s/mol.
4640 Processing CHEMBL4175914 in molecule.smi (4297/4695). Average speed: 0.12 s/mol.
4641 Processing CHEMBL4161860 in molecule.smi (4298/4695). Average speed: 0.12 s/mol.
4642 Processing CHEMBL4172510 in molecule.smi (4299/4695). Average speed: 0.12 s/mol.
4643 Processing CHEMBL4168710 in molecule.smi (4301/4695). Average speed: 0.12 s/mol.
4644 Processing CHEMBL4164186 in molecule.smi (4300/4695). Average speed: 0.12 s/mol.
4645 Processing CHEMBL4160790 in molecule.smi (4302/4695). Average speed: 0.12 s/mol.
4646 Processing CHEMBL4164524 in molecule.smi (4303/4695). Average speed: 0.12 s/mol.
4647 Processing CHEMBL4173258 in molecule.smi (4304/4695). Average speed: 0.12 s/mol.
4648 Processing CHEMBL4168617 in molecule.smi (4305/4695). Average speed: 0.12 s/mol.
4649 Processing CHEMBL4160694 in molecule.smi (4306/4695). Average speed: 0.12 s/mol.
4650 Processing CHEMBL462946 in molecule.smi (4307/4695). Average speed: 0.12 s/mol.
4651 Processing CHEMBL553245 in molecule.smi (4308/4695). Average speed: 0.12 s/mol.
4652 Processing CHEMBL4172401 in molecule.smi (4309/4695). Average speed: 0.12 s/mol.
4653 Processing CHEMBL1171719 in molecule.smi (4310/4695). Average speed: 0.12 s/mol.
4654 Processing CHEMBL4165513 in molecule.smi (4313/4695). Average speed: 0.12 s/mol.
4655 Processing CHEMBL4176125 in molecule.smi (4312/4695). Average speed: 0.12 s/mol.
4656 Processing CHEMBL4162070 in molecule.smi (4311/4695). Average speed: 0.12 s/mol.
4657 Processing CHEMBL2314746 in molecule.smi (4314/4695). Average speed: 0.12 s/mol.
4658 Processing CHEMBL4168934 in molecule.smi (4315/4695). Average speed: 0.12 s/mol.
4659 Processing CHEMBL4164418 in molecule.smi (4316/4695). Average speed: 0.12 s/mol.
4660 Processing CHEMBL453019 in molecule.smi (4317/4695). Average speed: 0.12 s/mol.
4661 Processing CHEMBL4173190 in molecule.smi (4318/4695). Average speed: 0.12 s/mol.
4662 Processing CHEMBL465678 in molecule.smi (4319/4695). Average speed: 0.12 s/mol.
4663 Processing CHEMBL4171637 in molecule.smi (4320/4695). Average speed: 0.12 s/mol.
4664 Processing CHEMBL4163761 in molecule.smi (4321/4695). Average speed: 0.12 s/mol.
4665 Processing CHEMBL4164862 in molecule.smi (4322/4695). Average speed: 0.12 s/mol.
4666 Processing CHEMBL4175494 in molecule.smi (4323/4695). Average speed: 0.12 s/mol.
4667 Processing CHEMBL4168299 in molecule.smi (4324/4695). Average speed: 0.12 s/mol.
4668 Processing CHEMBL4160394 in molecule.smi (4325/4695). Average speed: 0.12 s/mol.
4669 Processing CHEMBL4173389 in molecule.smi (4327/4695). Average speed: 0.12 s/mol.
4670 Processing CHEMBL4165471 in molecule.smi (4326/4695). Average speed: 0.12 s/mol.
4671 Processing CHEMBL4170793 in molecule.smi (4328/4695). Average speed: 0.12 s/mol.
4672 Processing CHEMBL4167398 in molecule.smi (4330/4695). Average speed: 0.12 s/mol.
4673 Processing CHEMBL4160151 in molecule.smi (4329/4695). Average speed: 0.12 s/mol.
4674 Processing CHEMBL4175274 in molecule.smi (4331/4695). Average speed: 0.12 s/mol.
4675 Processing CHEMBL4163678 in molecule.smi (4332/4695). Average speed: 0.12 s/mol.
4676 Processing CHEMBL4175003 in molecule.smi (4333/4695). Average speed: 0.12 s/mol.
4677 Processing CHEMBL4167127 in molecule.smi (4334/4695). Average speed: 0.12 s/mol.
4678 Processing CHEMBL4159880 in molecule.smi (4335/4695). Average speed: 0.12 s/mol.
4679 Processing CHEMBL4170530 in molecule.smi (4336/4695). Average speed: 0.12 s/mol.
4680 Processing CHEMBL4164981 in molecule.smi (4337/4695). Average speed: 0.12 s/mol.
4681 Processing CHEMBL4172883 in molecule.smi (4338/4695). Average speed: 0.12 s/mol.
4682 Processing CHEMBL4166464 in molecule.smi (4339/4695). Average speed: 0.12 s/mol.
4683 Processing CHEMBL4174372 in molecule.smi (4340/4695). Average speed: 0.12 s/mol.
4684 Processing CHEMBL4163016 in molecule.smi (4341/4695). Average speed: 0.12 s/mol.

5030 Processing CHEMBL4295126 in molecule.smi (4687/4695). Average speed: 0.12 s/mol.
5031 Processing CHEMBL4284475 in molecule.smi (4688/4695). Average speed: 0.12 s/mol.
5032 Processing CHEMBL4291697 in molecule.smi (4689/4695). Average speed: 0.12 s/mol.
5033 Processing CHEMBL4293155 in molecule.smi (4691/4695). Average speed: 0.12 s/mol.
5034 Processing CHEMBL4281066 in molecule.smi (4690/4695). Average speed: 0.12 s/mol.
5035 Processing CHEMBL4281727 in molecule.smi (4693/4695). Average speed: 0.12 s/mol.
5036 Processing CHEMBL4282558 in molecule.smi (4692/4695). Average speed: 0.12 s/mol.
5037 Processing CHEMBL4278260 in molecule.smi (4695/4695). Average speed: 0.12 s/mol.
5038 Processing CHEMBL4292349 in molecule.smi (4694/4695). Average speed: 0.12 s/mol.
5039 Descriptor calculation completed in 9 mins 43.564 secs . Average speed: 0.12 s/mol.

5040 total 35364

5041 drwxrwxr-x 1 root root 4096 May 30 2020 PaDEL-Descriptor

5042 drwxr-xr-x 1 root root 4096 Jul 4 18:17 __MACOSX

5043 -rw-r--r-- 1 root root 655414 Jul 4 18:17

acetylcholinesterase_04_bioactivity_data_3class_pIC50.csv

5044 -rw-r--r-- 1 root root 10410 Jul 4 18:17 bioactivity_data_preprocessed.csv

5045 -rw-r--r-- 1 root root 70334 Jul 4 18:17 bioactivity_data_raw.csv

5046 -rw-r--r-- 1 root root 8356701 Jul 4 18:27 descriptors_output.csv

5047 -rw-r--r-- 1 root root 122 Jul 4 18:17 mannwhitneyu_LogP.csv

5048 -rw-r--r-- 1 root root 120 Jul 4 18:17 mannwhitneyu_MW.csv

5049 -rw-r--r-- 1 root root 129 Jul 4 18:17 mannwhitneyu_NumHAcceptors.csv

5050 -rw-r--r-- 1 root root 128 Jul 4 18:17 mannwhitneyu_NumHDonors.csv

5051 -rw-r--r-- 1 root root 124 Jul 4 18:17 mannwhitneyu_pIC50.csv

5052 -rw-r--r-- 1 root root 310658 Jul 4 18:17 molecule.smi

5053 -rw-r--r-- 1 root root 395044 Jul 4 18:27 output.log

5054 -rw-r--r-- 1 root root 231 Jul 4 18:17 padel.sh

5055 -rw-r--r-- 1 root root 25768637 Jul 4 18:17 padel.zip

5056 -rw-r--r-- 1 root root 14209 Jul 4 18:17 plot_LogP.pdf

5057 -rw-r--r-- 1 root root 13057 Jul 4 18:17 plot_MW.pdf

5058 -rw-r--r-- 1 root root 35715 Jul 4 18:17 plot_MW_vs_LogP.pdf

5059 -rw-r--r-- 1 root root 14693 Jul 4 18:17 plot_NumHAcceptors.pdf

5060 -rw-r--r-- 1 root root 14181 Jul 4 18:17 plot_NumHDonors.pdf

5061 -rw-r--r-- 1 root root 14081 Jul 4 18:17 plot_bioactivity_class.pdf

5062 -rw-r--r-- 1 root root 15186 Jul 4 18:17 plot_ic50.pdf

5063 -rw-r--r-- 1 root root 95652 Jul 4 18:17 results.zip

5064 df3 : Unnamed: 0 molecule_chembl_id ... NumHAcceptors pIC50

5065 0 0 CHEMBL133897 ... 6.0 6.124939

5066 1 1 CHEMBL336398 ... 5.0 7.000000

5067 2 2 CHEMBL131588 ... 5.0 4.301030

5068 3 3 CHEMBL130628 ... 5.0 6.522879

5069 4 4 CHEMBL130478 ... 6.0 6.096910

5070

5071 4690 4690 CHEMBL4293155 ... 3.0 5.612610

5072 4691 4691 CHEMBL4282558 ... 3.0 5.595166

5073 4692 4692 CHEMBL4281727 ... 3.0 5.419075

5074 4693 4693 CHEMBL4292349 ... 5.0 5.460924

5075 4694 4694 CHEMBL4278260 ... 4.0 5.555955

5076

5077 [4695 rows x 9 columns]

5078 cat molecule.smi | head -5 :

5079 b'CCOc1nn(-c2cccc(OCc3ccccc3)c2)c(=O)o1\tCHEMBL133897\nO=C(N1CCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC1CC1\tCHEMBL336398\nCN(C(=O)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F)c1ccccc1\tCHEMBL131588\nO=C(N1CCCC1)n1nc(-c2ccc(Cl)cc2)nc1SCC(F)(F)F\tCHEMBL130628\nCSc1nc(-c2ccc(OC(F)(F)F)cc2)nn1C(=O)N(C)C\tCHEMBL130478\n'

5080 cat molecule.smi | wc -l :

5081 cat padel.sh :

5082 bash padel.sh :

5083 ls -l :

5084 df3_X : Name PubchemFP0 ... PubchemFP879 PubchemFP880

5085 0 CHEMBL130628 1 ... 0 0

5086 1 CHEMBL131588 1 ... 0 0

5087 2 CHEMBL336398 1 ... 0 0

5088 3 CHEMBL133897 1 ... 0 0

5089 4 CHEMBL130478 1 ... 0 0

5090

5091 4690 CHEMBL4293155 1 ... 0 0

5092 4691 CHEMBL4282558 1 ... 0 0

5093 4692 CHEMBL4281727 1 ... 0 0

5094 4693 CHEMBL4292349 1 ... 0 0

```

5095 4694 CHEMBL4278260 1 ... 0 0
5096
5097 [4695 rows x 882 columns]
5098 df3_X : PubchemFP0 PubchemFP1 ... PubchemFP879 PubchemFP880
5099 0 1 1 ... 0 0
5100 1 1 1 ... 0 0
5101 2 1 1 ... 0 0
5102 3 1 1 ... 0 0
5103 4 1 1 ... 0 0
5104 ... ... ... ... ...
5105 4690 1 1 ... 0 0
5106 4691 1 1 ... 0 0
5107 4692 1 1 ... 0 0
5108 4693 1 1 ... 0 0
5109 4694 1 1 ... 0 0
5110
5111 [4695 rows x 881 columns]
5112 df3_Y : 0 6.124939
5113 1 7.000000
5114 2 4.301030
5115 3 6.522879
5116 4 6.096910
5117 ...
5118 4690 5.612610
5119 4691 5.595166
5120 4692 5.419075
5121 4693 5.460924
5122 4694 5.555955
5123 Name: pIC50, Length: 4695, dtype: float64
5124 dataset3 : PubchemFP0 PubchemFP1 PubchemFP2 ... PubchemFP879
PubchemFP880 pIC50
5125 0 1 1 1 ... 0 0 6.124939
5126 1 1 1 0 ... 0 0 7.000000
5127 2 1 1 1 ... 0 0 4.301030
5128 3 1 1 1 ... 0 0 6.522879
5129 4 1 1 0 ... 0 0 6.096910
5130 ... ... ... ... ...
5131 4690 1 1 1 ... 0 0 5.612610
5132 4691 1 1 1 ... 0 0 5.595166
5133 4692 1 1 1 ... 0 0 5.419075
5134 4693 1 1 1 ... 0 0 5.460924
5135 4694 1 1 1 ... 0 0 5.555955
5136
5137 [4695 rows x 882 columns]
5138 X : PubchemFP0 PubchemFP1 ... PubchemFP879 PubchemFP880
5139 0 1 1 ... 0 0
5140 1 1 1 ... 0 0
5141 2 1 1 ... 0 0
5142 3 1 1 ... 0 0
5143 4 1 1 ... 0 0
5144 ... ... ... ... ...
5145 4690 1 1 ... 0 0
5146 4691 1 1 ... 0 0
5147 4692 1 1 ... 0 0
5148 4693 1 1 ... 0 0
5149 4694 1 1 ... 0 0
5150
5151 [4695 rows x 881 columns]
5152 Y : 0 6.124939
5153 1 7.000000
5154 2 4.301030
5155 3 6.522879
5156 4 6.096910
5157 ...
5158 4690 5.612610
5159 4691 5.595166
5160 4692 5.419075
5161 4693 5.460924
5162 4694 5.555955

```

```
5163 Name: pIC50, Length: 4695, dtype: float64
5164 X.shape : (4695, 881)
5165 Y.shape : (4695,)
5166 X.shape : (4695, 137)
5167 (3756, 137) (3756,)
5168 (939, 137) (939,)
5169 r2 : 0.3859207434145284
5170 Y_pred : [ 3.97692472  8.61330281  5.9074655  6.00882171  7.64959373  6.75971077
5171          6.04439075  6.10462978  5.89577688  6.30196671  6.25125997  5.94609156
5172          5.52287875  6.54680246  6.05329919  3.45847651  6.55019295  7.49100942
5173          3.71720516  6.00433894  5.32737199  6.47392691  4.85289026  5.43790482
5174          7.28673699  6.69160316  5.58728231  6.43549833  5.12419405  3.05327201
5175          5.11629699  8.15248632  9.06587062  6.74987949  5.88332405  4.16292774
5176          4.97257185  5.06027694  5.44041467  4.78335585  4.3267919  4.4061789
5177          6.64245889  7.64364185  3.69465343  6.54226787  6.83957573  8.61330281
5178          5.57491154  5.23040775  5.04196913  5.59020306  7.29536927  5.35691615
5179          5.5363934  7.74204389  5.88603741  4.6782657  8.35358788  5.92737655
5180          6.02630879  5.30620834  6.08987857  3.98075101  6.03276812  4.38535959
5181          4.28937058  6.10019021  5.67335522  5.44937055  8.17465085  6.02980327
5182          4.77438195  5.15759576  5.63239521  6.02630912  3.7392972  10.438221
5183          6.84081799  6.39730289  5.09013411  6.94323862  6.05329919  4.26480287
5184          5.48454233  6.74461503  6.03598841  6.94278256  5.75211799  5.78761296
5185          6.40745552  4.71311319  4.01272248  6.31371441  5.15593054  5.11875024
5186          4.73602426  4.87127351  5.09703707  6.2435387  3.89278394  7.86762975
5187          7.43019475  4.86371636  5.60354078  5.20039086  5.47322635  8.00581175
5188          5.65019291  6.67853683  7.77933579  6.02728546  5.36218707  6.17341956
5189          6.74347392  5.44033392  5.87536468  4.77651597  8.13784289  5.82769094
5190          5.57491154  5.25207971  6.52355568  7.22368533  3.89579461  9.06587062
5191          7.71758279  5.56614613  6.1266786  7.28279491  6.51263375  6.30141109
5192          4.23595403  6.95487918  6.22813828  6.27312351  6.68144121  5.85353532
5193          5.44682202  6.1106169  7.50664101  4.4469965  5.52445997  5.75055032
5194          6.48045223  6.37662305  5.36364691  5.12196457  5.85353532  7.22368533
5195          5.92737655  4.74685762  5.86198209  5.48181182  5.57839981  4.94451759
5196          5.86142561  4.80636427  5.92737655  6.93987661  5.37723745  6.49266213
5197          6.1622076  5.93738028  3.7889625  6.92719729  8.11031633  6.4046407
5198          5.53201158  8.05191943  5.15527385  5.13425689  5.04640804  5.11384313
5199          8.2477953  5.42655375  5.42608063  5.09463957  5.35272792  5.66819842
5200          7.36086779  5.42306562  7.69189437  4.76868042  6.06159752  4.87751244
5201          6.25936182  4.33755402  8.3749323  6.12681106  5.18783536  6.95262983
5202          5.0926525  7.64364185  5.01333331  5.29991155  5.00564746  5.09703707
5203          6.00289523  5.71212122  4.23041889  7.3520647  4.35781912  6.57998451
5204          6.93987661  7.24308458  5.12196457  5.12196457  3.21150792  5.49647296
5205          5.42608063  6.18364816  6.4165761  5.47479234  6.95586564  8.35358788
5206          5.26847821  6.335848  7.79152674  5.43537578  6.28954255  5.50928281
5207          6.77991672  5.89536893  7.96664077  5.23892616  6.08419547  6.95262983
5208          4.52283846  5.52287875  6.90904008  5.2409888  8.32357208  5.1716466
5209          6.56563263  6.74303961  6.59090902  4.30103  5.21675785  4.52664611
5210          5.01837424  6.88057434  6.61821689  5.95619952  6.09099038  4.47656439
5211          5.43695432  3.29943222  7.53237644  6.97983933  4.75896182  6.22213775
5212          5.96596288  5.51096651  6.1283456  5.19343249  6.86104276  6.18967511
5213          5.46464738  5.39405656  3.72502641  5.70567419  6.03912154  4.29539335
5214          5.25433348  4.96260859  4.95362412  4.50109026  5.68902573  6.09066149
5215          6.44076433  7.259461  5.80711122  6.4046407  6.16113122  5.98255097
5216          4.86445767  5.84930107  7.58676328  5.77043958  7.57053952  6.03236356
5217          6.28612425  5.20301718  5.12196457  5.29089338  6.91337162  5.54566504
5218          5.45315446  6.35994175  5.5835971  7.3170021  6.03598841  4.23136916
5219          6.81523587  5.26847821  8.35358788  6.08758535  4.79829289  5.2080631
5220          6.65541273  6.15076565  5.30620834  6.69096392  5.64898388  8.3749323
5221          5.32286487  6.46187672  4.71935364  5.99833253  5.78761296  3.71527333
5222          6.17195757  4.51533276  4.68974939  3.45168688  5.15723834  4.86371636
5223          7.38607689  5.02506645  4.02050985  7.81650401  6.32575162  4.74524467
5224          5.71643348  7.16684544  7.0247707  5.98834402  6.7736117  3.92478467
5225          7.03180679  5.30065974  6.33952735  7.27987236  6.84081799  5.40500888
5226          5.24712056  6.0098116  4.73569948  6.55826145  4.8989023  5.48932999
5227          7.84777043  5.85599053  4.78134372  7.65018244  7.3814121  4.96217945
5228          5.33183034  6.17386659  4.58475049  7.3814121  5.26964753  5.23123388
5229          8.61330281  10.70102458  7.25725576  7.32512485  5.20808324  5.46276037
5230          10.438221  6.58551727  6.10019021  5.35408287  5.91117237  4.75608268
5231          7.93801416  6.15799526  4.97093279  5.27670007  5.55168381  4.82467692
```


5232	6.24606904	7.34150265	5.16436961	4.56749527	5.01990855	6.76421156
5233	5.40226229	5.21977643	4.89310487	6.48535005	4.53668196	4.75605756
5234	5.51496947	5.54467359	5.2113788	6.70241763	7.92363186	6.46501107
5235	5.22019223	3.90019255	6.98130044	5.29611396	5.11417409	5.13782538
5236	5.35691615	6.39490422	4.89056272	7.3814121	5.7658998	5.39841672
5237	4.91132692	6.26070923	4.25235706	5.06279844	4.81383864	6.92735806
5238	3.98075101	6.68030788	4.2298285	5.79106084	6.4165761	5.75672757
5239	8.07992442	5.72508202	6.24803121	5.82639186	6.53880973	4.98600153
5240	5.28075357	5.70285255	5.97116784	8.05191943	7.77035617	5.47323155
5241	3.05771067	6.53880973	5.57354295	6.6185925	6.4165761	8.35358788
5242	5.02885303	3.89262507	5.38775977	6.40170459	5.73262295	6.24638462
5243	7.6892577	6.4737153	5.30254141	4.58475049	5.86177138	4.67070996
5244	6.62048461	6.46581411	5.52287875	5.79938151	7.88538901	5.53997042
5245	8.61330281	5.44041467	6.21117226	4.55610719	4.87630168	4.4476992
5246	4.47320043	6.7666587	6.73460297	5.96952981	4.86371636	8.3749323
5247	7.12253868	5.72132649	7.93098268	6.134552	4.82668754	5.60912286
5248	4.98132252	7.10175942	7.15747803	6.00601912	5.28269862	5.58261178
5249	4.99604419	7.6622319	7.50826107	7.259461	5.75141333	5.41198103
5250	3.62971081	5.80623807	4.02050985	6.16398573	6.14092559	5.56614613
5251	5.84844631	4.76194059	6.10272581	5.7770642	5.63555164	3.98075101
5252	8.03936081	7.0656168	6.46522341	4.16292774	5.90081029	7.3814121
5253	5.42132334	4.10004246	5.51786252	4.47672265	5.2830225	8.61330281
5254	6.05579298	7.43257325	6.01562918	4.94702404	6.54782505	3.7392972
5255	4.86371636	6.00934496	4.87515333	6.6185925	6.44176385	7.29536927
5256	4.79829289	5.65247807	3.7889625	4.78782329	10.44026117	7.32580698
5257	5.589498	6.56751851	4.02050985	5.86354095	5.09703707	4.88135532
5258	5.83053757	6.18580027	5.43271364	4.24021269	5.21380535	5.23892616
5259	5.21284528	3.78116706	4.59118188	5.23892616	6.69160316	8.3749323
5260	7.36333891	7.0650857	5.92737655	7.15747803	5.96379555	7.10455896
5261	6.75794906	5.38579531	5.38517647	7.64364185	6.45057331	6.024253
5262	5.12196457	6.00772982	5.63239521	8.04321787	5.81829275	7.46775963
5263	6.01184283	5.89773074	7.3520647	6.15890319	5.11264496	6.24803121
5264	6.7865187	6.1283456	5.63523499	7.25725576	7.58605125	5.0297358
5265	6.63223245	3.93826854	4.90883224	8.23654305	6.37934001	4.71127648
5266	6.28278604	4.95547862	7.03565733	6.10400046	5.49960919	5.51096651
5267	4.72796987	6.7736117	7.0650857	5.17291741	6.69160316	6.72356567
5268	5.21426147	7.89404656	7.65018244	5.78865193	8.02495602	5.55483751
5269	4.01239	5.17849074	4.70987854	5.96494867	4.79700492	6.02728546
5270	7.0656168	5.082394	3.89127034	6.1283456	6.17510835	7.50982027
5271	6.80938463	4.69277189	6.12400565	3.72670709	5.43722037	5.81542767
5272	4.992703	3.98605316	7.40888535	6.33130343	5.62898362	5.21448589
5273	4.53929844	6.08346222	7.13833277	5.01044595	6.8883166	5.98255097
5274	5.65149279	7.69017029	8.02495602	6.65953045	7.259461	5.25436666
5275	4.73602426	8.3749323	7.03565733	4.16769549	5.90803992	5.47141652
5276	6.18295363	5.32635446	3.01013539	6.23834804	6.64245889	4.86671581
5277	4.33354372	5.58350061	7.78625134	3.25073878	6.54772266	7.6622319
5278	5.0566058	5.99473953	6.82928757	5.95844547	5.082394	5.676232077
5279	5.64747801	5.83034828	6.4046407	6.35926476	6.74573381	6.1729194
5280	6.92859949	6.57013189	8.43929888	4.83562171	6.99574895	6.47057172
5281	5.35261393	6.4165761	4.77438195	5.55666338	7.81817856	6.4165761
5282	5.73866026	6.91758429	6.38050904	5.22729267	7.29064613	5.34082361
5283	5.57340608	5.75903607	4.84397442	4.19494593	6.91758429	4.73602426
5284	4.76861543	7.46337351	10.70102458	7.26458792	7.26293897	6.66987115
5285	1.10180095	7.3814121	6.09954136	6.1887255	6.04645166	5.42422682
5286	6.97412592	5.58684528	4.01695242	5.12672155	6.6633034	4.94158422
5287	6.58101011	5.3701793	6.03598841	5.77890703	5.93562996	4.98234271
5288	8.201408	8.54861123	4.90507082	7.53186717	6.1401881	4.62920666
5289	5.60419384	6.72356567	5.67427917	6.44176385	7.83621489	6.56712127
5290	5.31345053	6.39730289	5.082394	5.91613098	5.54656468	6.57013189
5291	6.46654694	4.93788482	3.96998278	6.5672075	6.58301639	5.48132929
5292	6.93974252	4.88545452	6.26408746	5.35418496	5.25268874	4.70187317
5293	7.3318255	4.70987854	7.53186717	5.29611396	4.6084684	7.12253868
5294	7.6622319	5.52044023	6.83896951	6.13034318	5.98718148	4.63930463
5295	4.92406998	4.58475049	4.80374221	5.47584881	5.56945171	6.77095552
5296	6.80076471	7.3520647	5.57223439	6.10401705	7.87120874	6.98926628
5297	5.36787681	4.67273522	6.88595394	5.46441833	6.90523916	4.46094911
5298	6.81429688	5.4363826	5.92737655	5.67918142	6.29868797	4.20353507
5299	5.67952429	5.13561297	6.55209673	6.43119662	5.38867496	5.16037177
5300	5.40504828	4.22872729	5.87536468	8.62140426	4.26514973	5.03764232

5301	5.71871074	4.75608268	8.3749323	5.26847821	4.75040879	7.7396694
5302	5.52287875	6.26408746	4.72054685	6.21042452	5.69016528	5.95861871
5303	8.37323206	5.46441833	6.24803121	4.75896182	7.92363186	4.02050985
5304	5.65356102	5.84405943	4.68971037	6.58876422	8.00581175	5.98606284
5305	6.09310661	4.70987854	6.40170459	4.93463418	6.09954136	4.61632391
5306	6.02728546	7.25725576	6.06474291	7.48130544	5.19343249	5.72069561
5307	8.23654305	5.04745753	5.25299004	5.98611824	5.39841672	10.21294103
5308	6.73010258	6.73460297	5.56614613	4.30307809	5.90527807	4.83476557
5309	5.57710896	5.79038542	4.39611739	6.56065988	5.61778599	10.39393427
5310	3.66119892	6.13742424	4.94940818	6.3401331	5.48454233	6.54772266
5311	5.9103217	7.64364185	5.66852647	7.9119013	5.42088668	5.67857548
5312	6.02728546	4.58602482	5.	6.05627831	6.71146785	5.08019884
5313	5.4968398	5.11583826	8.30648449	7.19370558	6.02728546	5.98730376
5314	4.73602426	5.88332405	5.31522616	7.30072946	4.01780677	6.12400565
5315	5.37926197	6.1401881	6.07373311	6.60532493	7.57635648	5.1811103
5316	6.1844222	5.94255726	5.28650205	6.94	5.72775234	4.90341584
5317	6.21481936	6.52255456	8.05191943	4.65798675	6.1247951	7.50137956
5318	6.66456685	5.45315446	7.25725576	6.13449193	4.8948483	5.66298974
5319	6.04410897	6.61623412	6.68030788	6.00601912	9.18983591	5.27248451
5320	7.09399573	4.27650393	7.29536927	5.79037707	7.48680739	4.04801748
5321	5.3946918	4.24442859	3.71787262	5.47322635	6.18689405	5.95199075
5322	5.87283816	7.34388708	6.5672075	6.98926628	6.45139996	6.86795973
5323	7.06653052	4.90507082	7.1581369	4.77409518	5.67643272	5.3750142
5324	5.90022991	5.18828416	4.8010092	5.94434394	5.1419207	7.12253868
5325	5.14982935	6.98926628	5.36224662	6.46026685	5.72169657	7.3516607
5326	5.35408287	6.91758429	5.964698]			

5327 X.shape (4695, 881)

5328 X.shape (4695, 137)

	Adjusted R-Squared	...	Time Taken
5329			
5330	Model	...	
5331	DecisionTreeRegressor	0.83	0.11
5332	ExtraTreesRegressor	0.83	6.10
5333	ExtraTreeRegressor	0.83	0.11
5334	GaussianProcessRegressor	0.83	6.75
5335	RandomForestRegressor	0.79	3.58
5336	XGBRegressor	0.78	1.07
5337	BaggingRegressor	0.77	0.44
5338	MLPRegressor	0.74	4.94
5339	HistGradientBoostingRegressor	0.61	1.64
5340	LGBMRegressor	0.61	0.23
5341	KNeighborsRegressor	0.57	3.15
5342	SVR	0.49	5.12
5343	NuSVR	0.49	3.77
5344	GradientBoostingRegressor	0.38	1.88
5345	Ridge	0.26	0.04
5346	RidgeCV	0.26	0.15
5347	LassoCV	0.26	2.84
5348	ElasticNetCV	0.26	2.95
5349	LinearRegression	0.26	0.07
5350	TransformedTargetRegressor	0.26	0.09
5351	HuberRegressor	0.25	0.35
5352	BayesianRidge	0.24	0.08
5353	LinearSVR	0.23	0.71
5354	LassoLarsCV	0.23	0.28
5355	LassoLarsIC	0.22	0.09
5356	SGDRegressor	0.22	0.10
5357	PoissonRegressor	0.21	0.09
5358	AdaBoostRegressor	0.17	0.50
5359	OrthogonalMatchingPursuit	0.16	0.04
5360	OrthogonalMatchingPursuitCV	0.16	0.10
5361	GammaRegressor	0.15	0.06
5362	GeneralizedLinearRegressor	0.15	0.07
5363	TweedieRegressor	0.15	0.08
5364	LarsCV	0.11	0.43
5365	Lars	-0.00	0.12
5366	Lasso	-0.04	0.05
5367	ElasticNet	-0.04	0.04
5368	DummyRegressor	-0.04	0.03
5369	LassoLars	-0.04	0.05

```
5370 PassiveAggressiveRegressor -0.71 ... 0.10
5371 KernelRidge -14.29 ... 0.98
5372 RANSACRegressor -1739426445758863245312.00 ... 0.57
5373
5374 [42 rows x 4 columns]
5375 Empty DataFrame
5376 Columns: [Adjusted R-Squared, R-Squared, RMSE, Time Taken]
5377 Index: []
5378 -----Starting phase 1 execution
-----
5379 -----Completed phase 1 execution
-----
5380 -----Starting phase 2 execution
-----
5381 -----Completed phase 2 execution
-----
5382 -----Starting phase 3 execution
-----
5383 -----Completed phase 3 execution
-----
5384 -----Starting phase 4 execution
-----
5385 -----Completed phase 4 execution
-----
5386 -----Starting phase 5 execution
-----
5387 -----Completed phase 5 execution
-----
5388
```