Section 1: General information

Materials sources:

All reagents for chemistry steps were obtained from Sigma or Acros. SuperFi DNA polymerase (Invitrogen), 2'-deoxyribonucleoside triphosphates (dNTP, set of dATP, dTTP, dGTP, dCTP, New England Biolabs), and T4 DNA ligase (New England Biolabs), were used as provided. Oligonucleotides (Integrated DNA Technologies) were obtained as desalted lyophilate and used without additional purification. FMOC-Cys(STmp)-OH, Sulfo-Cy5-azide were obtained from Sigma. Sulfo-Cy5-DBCO and monoBromobimane (mBBr) were obtained from Lumiprobe and Thermofisher, respectively. Filter plates (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE) and BIS-Tris propane were purchased from EMD Millipore. 40% Acrylamide/Bis (19:1) was purchased from Bio-Rad.

Note: mBBr should be stored at -80°C in DMF. DMF or DMSO solutions of this dye lose efficiency over time. It is recommended to do titrations to find the optimal dye concentration for staining, if it was stored for an extended period.

Buffers

• BIS-Tris propane ligation buffer (BTPLB): 50 mM NaCl, 10 mM MgCl₂, 1 mM ATP, 0.02% Tween 20, 10 mM bis-tris, pH 7.6

• BIS-Tris propane wash buffer (BTPWB): 50 mM NaCl, 0.04% Tween 20, 10 mM bis-tris, pH 7.6

• BIS-Tris propane breaking buffer (BTPBB): 100 mM NaCl, 10 mM ethylenediaminetetraacetic acid, 1% SDS, 1% Tween 20, 10 mM bis-tris, pH 7.6

• Click reaction buffer (CRB): 50% DMSO, DI water, 1M triethylammonium acetate, 0.04% Tween 20, pH 7.4. Note: Mix DMSO and DI water (smells fishy) and then adjust pH (7.4) by addition of 1M TEAA buffer.

- 2X-PBS: 0.4 g/L KCl, 0.48 g/L KH₂PO₄, 16 g/L NaCl, 2.88 g/L Na₂HPO₄ (anhydrous), pH 7.4.
- 2X-PBST: 2X-PBS, 0.2% Tween-20.
- Annealing buffer: 1 mM BTP, pH 7.6, 50 mM NaCl

Note: CRB was made fresh prior to each N3-hDNA click reaction

Oligonucleotide sequences

Name	Sequence (5' - 3')
ABM062	/5AmMC6/GTGGCACAACAACTGGCGGGCAAAC
ABM063	GCCGCCCAGTCCTGCTCGCTAC
ABM96	CGCCAGGGTTTTCCCAGTCACGACCAACCACCAAACCACAAACCCAAACCC CAAACCCAACACAACA
ABM99	GTGGCACAACAACTG
ABM100	CCTCTCTATGGGCAGTCGGTGATGTGGCACAACAACTGGCGGGCAAAC
CES1	GTTTTCCCAGTCACGAC
U6-Rev	GACTATCATATGCTTACCGT

Frag_Fwd- 1107[+]	/5Phos/GCCGCCCAGTCCTGCTCGCTTCGCTACATGGCAGAAGGA
Frag_Fwd-1107[-	/5Phos/TGATCCTTCTGCCATGTAGCGAAGCGAGCAGGACTGGGCGGCGG
Frag_2209/1306/ 2406/1506[+]	/5Phos/TCATTCTTCATGTTATAGAGCCCTACATTTCAATTCATAGAGCC
Frag_2209/1306/ 2406/1506[-]	/5Phos/GCGGGCTCTATGAATTGAAATGTAGGGCTCTATAACATGAAGAA
Frag_2604/1707/ 2802[+]	/5Phos/CGCAACCCTACGTACAGAAGGATGGAACCTCAATCTAAGAGGCA
Frag_2604/1707/ 2802[-]	/5Phos/CTTTGCCTCTTAGATTGAGGTTCCATCCTTCTGTACGTAGGGTT
Frag_1901/2A01/ Rev[+]	/5Phos/AAGCCTCCTAAGCCTGTTTGCCCGCCAGTTGTTGTGCCAC
Frag_1901/2A01/ Rev[-]	/5Phos/GTGGCACAACAACTGGCGGGCAAACAGGCTTAGGAGG
ABM99_2A07- Rev	GTGGCACAACAACTGGCGGGCAAACAGGCCCGGAGGGCTT
P5_Univ_Fwd-2	AATGATACGGCGACCACCGAGATCTACACTCTTTCCCTACACGACGCTCTTCC GATCTNNNNNNNNNGCCGCCCAGTCCTGCTCGCTTCGCTAC
Illumina Index 1	CAAGCAGAAGACGGCATACGAGATCGTGATGTGACTGGAGTTCAGACGTGTG CTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC
Illumina Index 2	CAAGCAGAAGACGGCATACGAGATACATCGGTGACTGGAGTTCAGACGTGTG CTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC
Illumina Index 3	CAAGCAGAAGACGGCATACGAGATGCCTAAGTGACTGGAGTTCAGACGTGTG CTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC
Illumina Index 4	CAAGCAGAAGACGGCATACGAGATTGGTCAGTGACTGGAGTTCAGACGTGTG CTCTTCCGATCTGTGGCACAACAACTGGCGGGCAAAC

Section 2: Methods

2A: General solid phase synthesis protocol

Compounds were synthesized on TentaGel resin using general SPS protocol described below.

Linker-1, used for FACS studies and DEL synthesis, was synthesized on 10 μ m TentaGel M NH₂ resin (Rapp-Polymere ,0.23 mmol/g). Linker-2, for mass analysis, was synthesized on 160 μ m TentaGel MB RAM resin (0.41 mmol/g). TentaGel rink amide resin (160 μ m, 0.41 mmol/g, 0.2 mmol, 50 mg, Rapp-Polymere) was transferred to a fritted spin-column (Mobicol Classic, large filter, 10 μ m pore size) and swelled in DMF (1 h, RT). FMOC was removed with 20% piperidine in DMF (3x resin volume after swelling, 500 μ L) at RT for 10 minutes, twice. It was then washed thoroughly with DMF, DCM and DMF, and successively coupled with either amino acids or peptoid units. In general, acids (5 times of resin capacity, 1.0 mmol) were pre-activated at RT for 5 minutes with DIC/Oxyma/Collidine (1.4/1.0/1.0 mmol) in DMF, added to the resin, incubated at 37°C for one hour, and washed with DMF, DCM (5 times each, 5x resin volume). FMOC was removed where applicable.

Figure S1: Linkers used in FACS and LCMS study



For peptoid units, bromoacetic acid (BAA) (1.0 M, DMF) and DIC (0.9 M) were added to the resin separately, vortexed, and incubated at 37°C for 1hr. Resin was washed thoroughly with DMF, DCM, and DMF and then sonicated in DMF for 2 minutes before further reactions. Amine (1.0 M, 1.5x resin volume, 500 µL DMF) was added successively and incubated at 37°C for 3 hrs., with agitation. *Note*: Too concentrated BAA+DIC solution had incomplete addition. Longer reaction time (~1hr) with lower conc resulted better yield.

Linker-2 was synthesized upon addition of Fmoc-Arg(Pbf)-OH, BAA, 1-Naphthylmethyl amine, BAA, 4bromobenzyl amine, Fmoc-Gly-OH, BAA, Propargyl amine, and Fmoc-EEAC, respectively, after swelling and FMOC removal.

Linker-1 was synthesized upon addition of Fmoc-Gly-OH, BAA, Propargyl amine, and Fmoc-EEAC respectively.

2B: STMP group removal, cyclization and staining with mBBr.

After synthesis of linear precursor was complete, resin was washed 3 times each with MeOH, DCM and DMF. Mixture of DTT and N-methylmorpholine base (100 mM each in DMF) was added (500 μ L for 50 mg, 10 μ m beads, 150 μ L for 0.5 mg of 10 μ m beads in plate), incubated for 5 min at RT, washed with DMF & DCM and repeated for two more times. Beads were washed 3 times each with DMF, 50% DMF-PBS and PBS buffer. It was suspended in PBST (pH = 7.6) and incubated at 37°C for 8-16 hrs. for cyclization. For large scale preparation *N*-Methylmorpholine (100 mM in DMF) was used for cyclization.

After desired time of cyclization, mBBr (150.0 μ L, 3.0 mM in DMF, 0.5 mg, 10 μ m bead) was added in filter plate (MultiScreen Solvinert 0.45 μ m Hydrophobic PTFE) and incubated at 37°C for one hour (9.0 mM, 2 hrs. when DNA tags are present). It was then washed with DMF, DCM, MeOH, suspended in PBST, and filtered into BD FACS tube for flow cytometry.

Figure S2: Standard protocol for OBOC thioether macrocyclization



2C: Copper based click (CuAAC) reaction to attach Cy5-azide dye and headpiece-DNA.

Cy5-azide dye was clicked to the alkyne in the linker region via CuAAC reaction before thiol deprotection, according to the Table **T2**. A similar procedure was followed for the azido-headpiece DNA (N3-hDNA).

In general, resin was suspended in freshly prepared CRB buffer (pH = 7.4) for one hour before the click reaction. CuSO₄-5H₂O (500 mM in water) and Tris[(1-benzyl-1H-1,2,3-triazol-4-yl)methyl]amine (TBTA, 50 mM in DMSO) were mixed in a 1:1 molar ratio, in CRB buffer, to obtain a blue colored solution. To this was added 50% of the required Na-ascorbate. The solution was then incubated for 5 min at 37°C to prepare the click-mix. A second solution containing the azide-click partner and the remaining Na-ascrobate was then added to the click-mix, vortexed, added to the resin, and incubated at 37°C for 2-4 hrs. After the reaction was complete, the resin was washed with organic solvent (DMF, DCM, MeOH), then extensively with aqueous buffer (BTP-WB & BTP-BB) and was suspended in BTP-BB (breaking buffer) overnight to remove copper salt before further reactions. BTP-BB solution turns blueish after overnight suspension.

For dye addition, DMSO solution of Cy5-N₃ was added (final conc 0.11mM) to the click-mix and incubated for 2 hrs. at 37°C.

Headpiece DNA was added to batches of 30.0 mg Linker-1 beads in 2.0 ml Bio-Rad spin column fitted with a 10 μ m filter. The click-mix was prepared according to Table **T1**, then incubated at 37°C for 5 min before being added to the resin. A solution of N₃-HDNA (3.0 mM, H₂O, 0.008 equiv. of resin capacity) was then added to the click-mix, vortexed, and incubated for 4 hrs. at 37°C.

Figure S3: General protocol to attach Cy5-azide dye and Azido headpiece DNA to the linker-alkyne



Table T1: General protocol for coupling Azido-HDNA with linker-1 beads via CuAAC reaction.

Azido-HDNA addition					
Reagents	Stock (mM)	equiv	mmols	amount	unit
Beads (10 uM) ~ loading 0.23			0.0069	30.00	mg
CuSO4 (H2O)	500	1.000	0.0069	13.80	ul
TBTA (DMSO)	50	1.000	0.0069	138.00	ul
Azido-peg-HDNA in TEAA buffer	3.1	0.008	0.0000552	17.81	ul
Na-Ascorbate (H2O)	500	6.000	0.0414	82.80	ul
CRB buffer				1747.59	ul
Total rxn vol				2000.00	ul

	Table T2: General	protocol for c	oupling Cy	5-azide dye	with linker l	beads via (CuAAC reaction.
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Cy5-N3 dye addition						
Reagents	Stock (mM)	equiv	mmols	Cy5(mM)	amount	unit
Beads (10 uM) ~ loading 0.23			0.000115		0.50	mg
CuSO4 (H2O)	500	1.000	0.000115		0.23	ul
TBTA (DMSO)	50	1.000	0.000115		2.30	ul
Cy5-N3 (DMSO)	12			0.11	1.38	ul
Na-Ascorbate (H2O)	500	6.000	0.00069		1.38	ul
CRB buffer					144.72	ul
Total rxn vol					150.00	ul

2D: General two-color staining protocol without a DNA tag

Cy5-azide dye was attached to the alkyne part of linear precursor via CuAAC reaction before thiol-protecting group was removed (Section **2C**). Click-mix was prepared for total amount of resin according to Table **T2**, incubated at 37°C for 5 min, added to the resin (for filter plates, 150 μ L, 0.5 mg/well) and incubated at 37°C for 2 hrs. Thiol-protecting STMP group was removed (Section **2B**) using 100 mM DTT-NMM, washed, and solvent exchanged to PBST buffer for cyclization. Resin was washed with 2X-PBS and re-suspended in

2X-PBS buffer and DMF solution of mBBr (final conc. 3.0 mM, 150.0 µL for 0.5mg, 10 µm beads) was added. It was incubated at 37°C for one hour before washing with DMF, DCM and DMF.

This general protocol was applied for staining control molecules and 64 scaffolds in the absence of DNA tags. For DNA-tagged control compound **2** & **3**, Cy5-azide dye (0.11 mM final conc. added 2 hrs. after N₃-HDNA addition) was clicked together with Azido-HDNA (0.002 equiv.), prior to thiol deprotection, at 37°C for 4 hrs. After thiol deprotection, the resin was transitioned to PBST, then a DMF solution of mBBr (final conc. 9.0 mM, PBST) was added and incubated for 2 hrs. at 37°C. It was then washed with MeOH, DCM and DMF.

For staining in the presence of DNA tags, please see Section 6.





2E: DNA Ligations

DNA fragments are ordered as pairs of single-stranded DNA oligonucleotides, which are then annealed to form double-stranded fragments. The individual oligos are re-suspended at 1600 μ M, mixed at equimolar ratios to 800 μ M, then diluted to 80 μ M in annealing buffer before being denatured and annealed (95°C, 2 min., -0.1°C/s to 25°C). The annealed oligos are mostly complementary but do have small 5' or 3' overhangs to permit directional ligation. The DNA fragments with complementary overhangs are then ligated to build the DNA barcode. Final ligation reactions included: 1X BTPLB, each dsDNA encoding fragment at an equimolar ratio to bead-bound HDNA, 2 μ I T4 DNA ligase per mg of beads. Incubated at RT, with gentle agitation, 4 hours.

Section 3: Two-color staining and fluorescence measurements of control compounds

3A. Titration of Cy5-azide dye: Control compound **3** (0.5 mg, 0.11 µmols, 10 µm TentaGel M NH₂ resin) was transferred to separate wells in a filter plate (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE) and suspended in CRB for one hour. Following general protocol described in section **2C**, click-mix solution was prepared in CRB according to Table **T2** and was added to each well (~150 µL). DMSO solution of Cy5-azide dye was added for final concentrations of (0.04 – 0.11 mM) and incubated for 2 hrs. at 37°C. Beads were washed, suspended in PBST, and filtered into BD FACS tube (~20,000 beads). Fluorescence intensity of these beads was measured (Red channel) to ensure it is under the linear range of flow cytometer. It appeared that the final Cy5 dye concentration of 0.11 mM is optimal and will be used in later studies.



Figure S5: Cy5-dye titration with compound 3.

3B. Optimization of mBBr concentration

Resin displaying control compound **2** (0.5 mg, 0.11 μ mols, 10 μ m TentaGel M NH₂ resin) was transferred to separate wells in a filter plate. The thiol-protecting STmp group was removed (Section **2B**) and the resin was washed and transitioned to PBST (pH = 7.6). A solution of mBBr (23.0 mM, in DMF) dye was added

to each well for final concentrations of 1.0 - 7.0 mM. The plate was then incubated at 37°C for one hour. It was washed with DMF, DCM, MeOH, and DMF-PBST (50%) buffer, re-suspended in PBST and filtered into BD FACS tubes (~20,000 beads) for FACS analysis (BV510).



Figure S6: Monobromobimane (mBBr) dye titration with compound 2.





After staining with mBBr, control compound **2**, which represents a linear model, fluoresces brightly in the green channel while compound **3** (cyclic model) shows almost no fluorescence (Figure **S7**, Panel C vs D) indicating high specificity of mBBr with free thiols but not with thioethers. In contrast, compound **2** & **3** both fluoresce brightly after staining with Fluorescein-5-Maleimide (FITC, panel I) which indicates FITC binds to the beads nonspecifically and therefore cannot be used in this assay. The sulfo-CY5 dyes tested did not show non-specific binding to the resin.

For two color staining, resin displaying compound **2** was first stained with Cy5 dye, followed by thiol deprotection and staining with mBBr. In the presence of Cy5, a higher amount of mBBr (3.5 mM, Panel H) was required to achieve similar fluorescence intensity without the Cy5 dye, although fluorescence compensation was not required. Under identical staining conditions as with mBBr, compound **2** fluoresces 100-fold more than compound **3** (Panel J).

Note: It was observed that, for fresh mBBr, a lower concentration (1.0- 3.0 mM) is optimal. However, over time mBBr loses efficiency and titration should be repeated to find the optimal dye concentration.

Section 4: Cyclization progress of DDA scaffold via LCMS/FACS

Scaffold **DDA** was synthesized on both 10 (linker-1) & 160 (linker-2) µm beads separately in spin columns (10 µm filter) after adding FMOC-Cys-(STmp)-OH, 2-(Chloromethyl)oxazole-4-carboxylic acid (3x) and 3-(Chloromethyl)-benzoic acid respectively following the general SPS protocol (Section **2A**). 3-methoxypropyl amine was used in all **X1-3** position (Figure S8A & B). After the linear precursor was synthesized, it was transferred to two separate filter plates (0.5 mg /well) and thiol protection was removed. Beads were washed with DMF, DCM, DMF-PBS (50%), and finally suspended in PBST.

Figure S8A: FACS analysis with 10 µm beads



Figure S8B: LCMS analysis with 160 µm beads



The ring closure process was monitored from point t= 0, onwards. After thiol exposure, mBBr (3.0 mM, 150 μ L for 0.5mg /0.1 μ mol of 10 μ m TentaGel resin) and benzyl bromide (1.0 M, 150 μ L for 0.5mg /0.2 μ mol of 160 μ m TentaGel resin) were added separately at t = 0, 2, 4, 6, 8 &16 hrs. and incubated at 37°C for one hour. After 16 hrs., the 160 μ m beads were TFA-cleaved (90% TFA, 2.5% TIPS, 2.5% thioanisole and 5% DCM, 2hrs, RT) and analyzed by LCMS, while 10 μ m beads were passed through a 35 μ m cells strainer and analyzed by FACS to measure fluorescence. As expected, at t = 0 hrs., mostly benzylated linear material (Figure **S8B**, Mw 1825) was obtained, while at t = 16 hrs., cyclo-**DDA** was obtained in major quantity. As cyclization progresses over time, absorbance for linear material (RT = 9.5 min) tend to diminish as expected.



At t = 0, major ion corresponds to benzylated linear material.

At t = 16 hrs., cyclo-DDA was obtained in major quantity.



Cyclization progress of DDA from t = 2 - 16 hrs.



4C: Investigate stability of the sulfhydryl group after 16hrs. of incubation



Due to concerns about general thiol oxidation occurring during 16 hours of cyclization, which would prevent mBBr addition and falsely indicate cyclization, an experiment was designed to test the stability of the sulfhydryl group. An acetylated version of the scaffold DD-STmp was synthesized on 160 µm beads (linker

2) after adding FMOC-Cys-(STmp)-OH. 2-(Chloromethyl)oxazole-4-carboxylic acid (3x) was the backbone unit, while 3-methoxypropyl amine was used in the amine positions. After the final amine addition, the compound was acetylated to prevent cyclization. The beads were then transferred to a filter plate (0.5mg/well), thiol protection was removed, and the resin was incubated at 37°C in PBST for 16 hrs. After 3 washes with PBST, the resin was treated with DMSO solution of benzyl bromide (final conc 1.0M, PBST) at 37°C for one hour, cleaved with TFA, and analyzed by MALDI. The data indicate that the sulfhydryl group remains intact and is able to react with the benzyl bromide, as observed below.



Section 5: Cyclization efficiency of 64 PICCO scaffolds



Synthesis & characterization of 64 scaffolds: 64 PICCO scaffolds (3.5-mer) were synthesized, in parallel, on 10 (linker-1) & 160 (linker-2) µm TentaGel resins in separate filter plates (MultiScreen Solvinert 0.45 µm Hydrophobic PTFE). Linkers 1 & 2 were functionalized with FMOC-Cys-(STmp)-OH, then acid D, and distributed into the filter plate (0.5 mg / well). Scaffold synthesis was completed by iterative couplings of the various acids (A-D, preactivated for 5 minutes with oxyma/DEC/collidine, 1 hr., 37°C) and 3-methoxypropyl amine (1.0 M, 3 hrs., 37°C). Cy5-azide was then clicked onto the 10 µm resin only, followed by copper salt removal with BTP-BB, overnight. Thiol protection was then removed on both 10 µm and 160

 μ m resins with 100 mM DTT and 100 mM NMM, in DMF solution (3 x 5 min) at RT. The beads were then washed with DMF, DCM, and DMF-PBS, then suspended in PBST (pH = 7.6) buffer and incubated for 8 hrs. at 37°C, for cyclization. With synthesis complete, the 10 μ m beads were then washed with and transitioned to PBST, labeled with mBBr (3.0 mM, 37°C, 1 hr), washed with DMF, DCM, and DMF-PBS buffer, then resuspended in PBST and filtered (35 μ m) into 64 FACS tubes for FACS analysis. The 160 μ m beads, meanwhile, were washed, suspended in DMF for one hour, and cleaved (90% TFA, 2.5% TIPS, 2.5% thioanisole and 5% DCM) for mass analysis.

	1	2	3	4	7	8	9	10
К	AAA	ABA	ACA	ADA	AAB	ABB	ACB	ADB
L	BAA	BBA	BCA	BDA	BAB	BBB	BCB	BDB
М	CAA	CBA	CCA	CDA	CAB	CBB	CCB	CDB
Ν	DAA	DBA	DCA	DDA	DAB	DBB	DCB	DDB
0	AAD	ABD	ACD	ADD	AAC	ABC	ACC	ADC
Р	BAD	BBD	BCD	BDD	BAC	BBC	BCC	BDC
Q	CAD	CBD	CCD	CDD	CAC	CBC	CCC	CDC
R	DAD	DBD	DCD	DDD	DAC	DBC	DCC	DDC

Table T4: Ring closure summary (FACS & LCMS) of 64 Scaffolds

Note1: "3.5-mer" means the scaffold has four acids and three amines, but the first acid is always acid D. "2.5-mer means" scaffold has three acids and two amines.

Note2: Although 160 µm beads had 8 hrs. incubation time, cyclization may continue during and after TFA cleavage reaction. However, cyclization was frozen for the selected two-color population on 10 µm bead after mBBr addition, but continued during TFA cleavage. This indicates that few scaffolds have more conformational constraint than others and need more time to cyclize.

Note3: Some scaffolds cyclized as it is (3.5-mer to 3.5-mer) and some has incomplete acid addition residues, which in most cases also cyclized (2.5-mer).

5A: Ring closure analysis - summary of 64 scaffolds:

Each scaffold is analyzed by how much linear starting material (3.5-mer) is left after cyclization for 8 hrs. If a scaffold had 90% cyclization, it was considered complete. If it had 40% or more linear material left, it was considered incomplete. Due to incomplete synthesis reactions, some "2.5-mer" scaffolds were generated (ABA, ABB, BBA). Regardless, these compounds mostly cyclized as well. Ring closure is primarily reviewed for 3.5-mer compounds and examined that any 2.5-mer linear fragments contributed as false positive. In the LCMS analysis, combined area of all the cyclic compounds are compared against combined area of all the linear compounds.

Table T5: LCMS analysis of ring closure of 64 scaffolds

				cyclization status	linear SM		nature	
En- try	Posi- tion	Scaffold	FACS	mass-spec	left(%)	cyclic: linear	of scaffold	comment
1	K1	AAA	incomplete	complete	7.5	93.0:7.0		
2	K2	ABA	complete	complete				
3	K3	ACA	incomplete	complete				
4	K4	ADA	complete	complete	3.8	96.2:3.7		
5	K7	AAB	complete	incomplete	70.7	58.5: 41.4	difficult to cyclize	
6	K8	ABB	complete	incomplete	17.2	85.4: 14.7		
7	K9	ACB	incomplete	incomplete	28.8	69.6:20.1		
8	K10	ADB	incomplete	incomplete	20.9	82.6: 17.3		
9	L1	BAA	incomplete	complete				
10	L2	BBA	complete	complete				
11	L3	BCA	complete	complete				
12	L4	BDA	complete	complete				
13	L7	BAB	complete	complete	9.7	91.0: 8.9		
14	L8	BBB	complete	complete				
15	L9	BCB	complete	complete	4.7	95.5:4.5		Linear-2.5 mer
16	L10	BDB	complete	incomplete	30.8	76.4: 23.6		
17	M1	CAA	complete	complete				
18	M2	CBA	complete	complete				
19	M3	CCA	complete	complete				
20	M4	CDA	complete	complete				
21	M7	CAB	complete	incomplete	45	69.0: 31.0	difficult to cyclize	
22	M8	CBB	complete	incomplete	33.4	74.7: 25.2		linear- 3.0 mer
23	M9	ССВ	incomplete	incomplete	66.7	60.0: 40.2	difficult to cyclize	
24	M10	CDB	complete	incomplete	27.2	78.5: 21.4		
25	N1	DAA	complete	complete				
26	N2	DBA	complete	complete				
27	N3	DCA	complete	complete				
28	N4	DDA	complete	complete				
29	N7	DAB	complete	incomplete	27.7	78.4: 21.6		
30	N8	DBB	complete	incomplete	34	74.6: 25.4		
31	N9	DCB	incomplete	incomplete	13.4	88.1: 11.8		
32	N10	DDB	complete	complete				
33	01	AAD	incomplete	complete				

1	1	1	1		1	1	1	1
34	O2	ABD	complete	complete				
35	O3	ACD	incomplete	complete				
36	O4	ADD	complete	complete				
37	07	AAC	complete	complete	2	98.1: 2.0		
38	O8	ABC	complete	complete				
39	O9	ACC	complete	complete				
40	O10	ADC	incomplete	complete	5	95.2: 4.8		
41	P1	BAD	complete	complete				
42	P2	BBD	complete	complete				
43	P3	BCD	complete	complete				
44	P4	BDD	complete	complete				
45	P7	BAC	complete	complete				
46	P8	BBC	complete	complete				
47	P9	BCC	complete	complete				
48	P10	BDC	incomplete	complete				
49	Q1	CAD	complete	complete				
50	Q2	CBD	complete	complete				
51	Q3	CCD	complete	complete				
52	Q4	CDD	complete	complete				
53	Q7	CAC	incomplete	complete				
54	Q8	CBC	complete	complete				
55	Q9	CCC	incomplete	complete				
56	Q10	CDC	incomplete	complete				
57	R1	DAD	complete	complete				
58	R2	DBD	complete	complete				
59	R3	DCD	complete	complete				
60	R4	DDD	complete	complete				
61	R7	DAC	complete	complete				
62	R8	DBC	complete	complete				
63	R9	DCC	complete	complete				
64	R10	DDC	complete	complete				

For fluorescence and LCMS data, please see section 9.

Section 6: Monitor on-resin cyclization progress in presence of DNA

To test for inhibition of macrocyclization by the encoding DNAs, cyclization progress was measured on resins that displayed full-length barcodes. Compounds **DDD**, **DDA**, **DDE** and **EBB** were synthesized on 10 & 160 µm beads (~5.0 mg). Headpiece DNA (0.008 equiv.) & 1,3-azidopropane (1.5 equiv., added two hours after azido-HDNA addition) were clicked together via a CuAAC reaction, and a full length, test-DNA tag was ligated onto the 10 µm beads. After linear precursor synthesis was complete, Cy5-DBCO was attached (final conc. 0.11mM, 150 µL CRB buffer, for 0.5 mg, 10 µm beads, ON, 37°C) via SPAAC reaction in a filter plate. The thiol-protecting STMP group was then removed and the compounds were cyclized for 16 hrs. at 37°C. The 10 µm beads were then treated with mBBr (final conc. 9.0 mM, 150 µL PBST, 2 hrs., 37°C) while the 160 µm beads were treated with benzyl bromide (1.0 M, 150 µL PBST, 2 hrs., 37°C) to freeze cyclization during or after TFA cleavage. DNA tags from the 10 µm beads were then PCR-amplified and Sanger sequenced. Ring closure status was then analyzed by FACS and MALDI.





Figure S11: DNA tag amplification of compounds DDD, DDA, DDE and EBB from 10 µm beads (1500 beads) in two replicates followed by controls (+ve, -ve) and Sanger sequencing results.



Test-DNA tags of these beads were amplified (Table **T7**, 1st PCR), purified (5.0 μ L) by native PAGE gel extraction (6%, 1 x TBE, 4 W, 60 min), with 1X SYBR Gold staining. Gel slices containing 167bp DNA products were excised and suspended in DI water (50.0 μ L) in a clean tube overnight. The samples were then centrifuged (5 min, 10,000 RCF), and the supernatants were transferred to clean tubes, diluted 1:10000 in BTPWB, and used as template for Sanger-primer-addition PCRs. The samples were again gel purified by native PAGE gel extraction (233bp DNA), suspended in DI water, centrifuged, and sent for Sanger sequencing (GENEWIZ).

All four samples had same test-DNA tag. They are shown below.

Expected DNA sequence :

1107[+], 2209[+], 1306[+], 2406[+], 1506[+], 2604[+], 1707[+], 2802[+], 1901[+], 2A01[+], 2

Found sequence as expected. All 4 samples had same test DNA tag below.

Position: 1																																			17	l bp
Reference Coordinates	20		30			40			50			60			70			8	0			90			100			110			12	20		130		
▶ Translate ▶ Consensus	CTA	CATGO	GCAG	AAGG	ATC.	ATTO	ттс	ATG	TAT	AGA	GCC	СТА	CATT	TCA	A T T	CAT.	AGA	GCCC	GCA	ACC	сти	A C G T	FAC.	GAA	GGA	A T G G	AAC	стс	TAA	стаа	GAO	GCA	AGC	стсс	TAAG	C
Test DNA Tag.seq(1>111) → ▼Reverse Read.ab1(16>140) ←		ATGO	GCAG	AAGG	ATC.	ATTO	ттс	ATG	TTAT	AGA	бСС	ста	CATT	TCA	ATT	С А Т .	AGA	6 6 6 6	GCA	ACC	сти	A C G T	FAC.	A G A J		A T G G	AAC	стс	AAT	стаа	6 . 6	GCA	AGC	стсс	TAA	٦
	M	Iw	M	M	Ŵ	M	M	Ŵ	W	M	M	M	M	M	M	W	W	W	Ŵ	W	W	Ŵ	M	Ŵ	Ŵ	M	M	\mathcal{M}	\sim	M	XXX	XX~	7			
\blacksquare Forward Read.abl(20>145) \rightarrow								Ŵ	<u>~00</u>	\mathcal{A}	α^{\sim}	XXX	XV	ν _χ	Ŵ	χ	W	W	Ŵ	Ŵ	W	W	M	W	W	M	M	M	M	Ŵ	Ŵ	W	Ŵ	Ŵ	Ŵ	M
								T 6 1	ΤΑΤ	AGA	GCC	CTĂ	CATT	TNA	ATT	CAT	AGA	6 C C C	GCA	ACC	CTI	A C G T	C A C	GA	GG	TGG	AAC	CTC	AAT	СТАА	GAO	GCA	AGC	стсс	TAAG	C



6A: Mass analysis of compounds DDD, DDA, DDE and EBB



Section 7: Synthesis & quality control of OBOC thioether macrocyclic DEL for ring closure.



Position 1

	1st amine-acio	ł											
	2401	2402	2403	2404	2405	2406	2407	2408	2409	2410		1309	1310
	H ₂ N Br	H ₂ N	H ₂ N~~_0~	H ₂ N	H ₂ N	H ₂ N	NH ₂	HNNNH	H ₂ N N	нуун		H ₂ N	H ₂ N F
1301	HOLON										2401		
1302	HOUCI										2402		
1303	HO CI										2403		
1304											2404		

Position 2

	2nd amine-ad	cid									_		
	2601	2602	2603	2604	2605	2606	2607	2608	2609	2610		1509	1510
	H ₂ N~~~ ⁰ ~	H2N	H ₂ N	H ₂ N H	Н₂№	H ₂ N	H ₂ N	H ₂ N	H ₂ N CF ₃			F ₃ C NH ₂	^{NH2}
1501											2601		
1502		HOLONCI			HOUTCI						2602	HO (R) (E) CI	
1503											2603		
1504											2604		

Position 3

:	Brd amine-aci	d											
	2801	2802	2803	2804	2805	2806	2807	2808	2809	2810		1709	1710
	H ₂ N	H ₂ N_OH	H ₂ N N	H ₂ N	H ₂ N 0	(R) NH ₂	NH ₂	H ₂ N	H ₂ N	O NH2		H ₂ N H ₂ N	H ₂ N (S)
1701	HO L S										2801		
1702	HOUCI										2802		
1703	но (S) СІ										2803		
1704	HO (R) Br										2804	ОН	CT OH

Synthesis & analysis: Linker-**1** was synthesized on 25.0 mg of 10 µm TentaGel amine beads, FMOC-Cys(STmp)-OH and acid **D** were then added, in succession. Azido headpiece-DNA and 1, 3-diazidopropane

were attached via CuAAC reaction following general method **2C**. The beads were then distributed into a filter plate (0.5 mg/ well, 48 wells, Millipore MultiScreen Solvinert 0.45 μ m Hydrophobic PTFE). Subsequently, FWD primer along with 11xx-22xx primers were ligated, beads were pooled and redistributed. Amines (1.0 M, 150.0 μ L, 3 hrs., 37°C) were reacted first, followed by acid additions for each position **X1-3** (Acid/DIC/Oxyma/Collidine: 80/126/80/80mM, pre-activated, 150.0 μ L, 3hrs., 37°C) following the general scheme **7A**. Beads were then washed (150.0 μ L, DMF, DCM, DMF, BTP-WB) and suspended in BTP-WB overnight before encoding.

X1-3 positions were encoded with primers 13xx-24xx, 15xx-26xx and 17xx-28xx, respectively. In general, an encoding oligonucleotide ligation mixture containing T4 DNA ligase (15000 U) in BTP-LB (1.35X) was prepared and aliquoted into all plate wells (110 μ L). Stocks of \approx 13XX[±] (Table **T5**) and \approx 24XX[±]were annealed and then added to the appropriate wells (final conc for each codes ~10mM, total vol 150uL) the plate was sealed with adhesive foil, and incubated with agitation (4h, RT, 800 rpm).

After each ligation, beads were transitioned to and equilibrated in DMF overnight before the chemistry steps. The library- id (1901-2A07) and reverse primer were then ligated to complete the DNA barcodes. The beads were then washed with and equilibrated with BTP-WB buffer, overnight. An aliquot of the library (~5.0 mg) was transferred to a fritted spin-column (Bio-Rad, large filter, 10- μ m pore size) and re-suspended in CRB, DMSO solution of Cy5-DBCO (final conc 0.11 mM, 150uL) was added and incubated at 37°C for overnight (2hr also works). The beads were then washed with BTPWB, DMF, and DCM before resuspending in DMF for overnight. The thiol-protecting STmp group was then removed (100.0 mM DTT-NMM in DMF, 500 μ L, 3x, RT). The beads were then suspended in PBST (1.00 ml) and incubated at 37°C to monitor cyclization. After 8, 12 & 16 hrs., aliquots of beads were transferred to a filter pate, stained with mBBr (9.0 mM, DMF, 37°C, 2hrs) , and analyzed by flow cytometry. Beads that have higher fluorescence intensities than control-**3** (due to incomplete cyclization) were separated and collected.

Sorted beads were transferred from the FACS collection tubes to clean centrifuge tubes (0.2 mL) and concentrated (to ~5.0 μ L). Encoding DNA tags were amplified (Table **T7**, 1st PCR) and purified (5.0 μ L) by native PAGE gel extraction (6%, 1 x TBE, 4 W, 60 min). Gel slices containing 167bp DNA products were excised and suspended in DI water (50.0 μ L) in a clean tube overnight. The samples were then centrifuged (5 min, 10,000 RCF), transferred to a clean tube, diluted to (1:10000 in BTPWB), and used as template for Illumina primer addition PCRs. Illumina index primers, along with the P5-univ-FWD primer, SuperFi buffer, SuperFI DNAP, and dNTP mix were premixed, 1.0 μ L of the template from the 1st PCR was added, and the mixture was thermally cycled (Table **T7**). The samples were again gel purified (289bp DNA), eluted with DI water, and deep sequenced.

Table T6. Oligonucleotide sequence lookup table.

Overhangs

Coding Sequences

Overhang #	Sequence	Identifie	r # Sequence	Identifier #	Sequence
≈X1XX[+]	/5Phos/ATGG	≈1X01[+] AAGAGAGG	≈2X01[+]	AGTTTCAG
≈X1XX[-]	/5Phos/TGA	≈1X01[-] ССТСТСТТ	≈2X01[-]	CTGAAACT
≈X2XX[+]	/5Phos/TCA	≈1X02[+] ACGGAGCA	≈2X02[+]	AACCTCAA
≈X2XX[-]	/5Phos/AAC	≈1X02[-] TGCTCCGT	≈2X02[-]	TTGAGGTT
≈X3XX[+]	/5Phos/GTT	≈1X03[+] ACAAAGAG	≈2X03[+]	AATCCCAT
≈X3XX[-]	/5Phos/TAG	≈1X03[-] CTCTTTGT	≈2X03[-]	ATGGGATT
≈X4XX[+]	/5Phos/CTA	≈1X04[+] AAGGAGGT	≈2X04[+]	AACCCTAC
≈X4XX[-]	/5Phos/GAA	≈1X04[-] ACCTCCTT	≈2X04[-]	GTAGGGTT
≈X5XX[+]	/5Phos/TTC	≈1X05[+] AGAAAGCA	≈2X05[+]	ATCCTCTC
≈X5XX[-]	/5Phos/GCG	≈1X05[-] TGCTTTCT	≈2X05[-]	GAGAGGAT
≈X6XX[+]	/5Phos/CGC	≈1X06[+] ATAAAGGT	≈2X06[+]	ATTCTCCG
≈X6XX[-]	/5Phos/AAC	≈1X06[-] ACCTTTAT	≈2X06[-]	CGGAGAAT
≈X7XX[+]	/5Phos/GTT	≈1X07[+] ATAGAAGG	≈2X07[+]	CGCCTTCA
≈X7XX[-]	/5Phos/TAG	≈1X07[-] CCTTCTAT	≈2X07[-]	TGAAGGCG
≈X8XX[+]	/5Phos/CTA	≈1X08[+] ATGGGAGT	≈2X08[+]	CGTTCCTG
≈X8XX[-]	/5Phos/AGGC	≈1X08[-] ACTCCCAT	≈2X08[-]	CAGGAACG
		≈1X09[+] GCAAAGGA	≈2X09[+]	CTCTCCAC
		≈1X09[-] TCCTTTGC	≈2X09[-]	GTGGAGAG
		≈1X10[+] TTGAGGAT	≈2X10[+]	TCCTCTTA
		≈1X10[-] ATCCTCAA	≈2X10[-]	TAAGAGGA

Primers

PCR Primer #	Sequence
≈0001[+]	/5Phos/GCCGCCCAGTCCTGCTCGCTTCGCTAC
≈0001[-]	/5Phos/CCATGTAGCGAAGCGAGCAGGACTGGGCGGCGG
≈0901[+]	/5Phos/GCCTGTTTGCCCGCCAGTTGTTGTGCCAC
≈0901[-]	/5AmMC6/GTGGCACAACAACTGGCGGGCAAAC

Table T7: PCR amplification of encoding DNA tags from beads.

1st PCR: Amplification of encoding DNA tags from beads					
rxn volume:	50	total rxns:	6		
reagent	vol	stock	MM volume	Cycle:	
initial vol	10		60		
5X SuperFi Buffer	10.0	5X	60.0	1	98°C, 30 sec
0.2 mM dNTP Mix	1.0	10 mM	6.0	2	98°C, 10 sec.
0.3 μM ABM99-2A-07*	1.5	10 uM	9.0	3	46°C, 10 sec.
0.3 μM ABM063	1.5	10 uM	9.0	4	72°C, 15 s
SuperFi DNAP	0.5	2U/ul	3.0	5	Goto 2, 25 times
ddH20	25.5	ddH20	153.0	6	4° hold
total	50.0	total	300.0		
*library specific rev primer					

Table T8: NGS sample preparation- addition of Illumina index primer

2nd PCR- add illumina rev-index and fwd primers						
rxn volume:	50	total rxns:	9			
reagent	vol	stock	MM volume		Cycle 2:	
5X SuperFi Buffer	10.0	5X	90.0		1	98°C, 2 min
0.2 mM dNTP Mix	1.0	10 mM	9.0		2	98°C, 10 sec.
0.3 μM P5 Univ Fwd2	1.5	10 uM	13.5		3	36°C, 10 sec.
0.3 μM Index Rev (1-4)*	1.5	10 uM			4	72°C, 15 s
SuperFi DNAP	0.5	2U/ul	4.5		5	Goto 2, 25 times
DNA Template (1k & 10k)fold diluted	1.0				6	4° hold
ddH20	34.5	ddH20	310.5			
total	50.0	total	427.5			
*Illumina index						

1st PCR: 25 Cycles







Figure S12: Fluorescence readout of DNA-linked control-**3**. Methionine-DNA-CY5 beads were treated with mBBr and analyzed by FACS. This is a negative control for analyzing OBOC macrocyclic DEL through a flow cytometer.



Figure S13: Fluorescence readout of beads from the macrocyclic DEL. After cyclization, beads were stained with Cy5-DBCO and MBBR (9.0 mM) and analyzed by FACS.



Sorting result: Beads that appeared in the cyclic region (MBBR/Cy5+) were collected and their encoding tags were deep sequenced.



For sequencing analysis of naïve and FACS-sorted beads, please see Sections 10 & 11, respectively.

Figure S14: (A) After deep sequencing, difficult to cyclize scaffolds were arranged by count (up to 5 copies, 74 scaffolds). Each line indicates a combination of three acids at position X1-3 for a scaffold along with its molecular ID (left) and the number of times it was present in the collected pool (right). (**B**) Acids A - G and amines were used in position X1-X3 to construct DEL scaffolds. 4% of DEL members were capped with acid H & I to keep them as linear controls for FACS analysis.



Section 8: FACS & LCMS analysis of 64-scaffolds

Fluorescence data analysis of 64 PICCO scaffolds after cyclization

Fluorescence readouts were recorded for each of the 64 scaffolds. Status of ring closures were determined by FACS and cross-referenced with mass spectra to see if there is any linear starting material remaining. The goal was to ultimately gauge the state of cyclization from FACS data by locating the majority of the bead population, without cleaving compounds from beads.

Each FACS plot is divided into 4 quadrants; Q1-Q4. After cyclization and two dye additions, if the majority of the bead population for a particular scaffold stays in Q1 (Cy5 +, MBBR -), cyclization will be considered as complete. If the scaffold does not cyclize efficiently, it will have unreacted thiol groups and will be present in Q2 (Cy5 +, MBBR +), as it will pick up both dyes. Negative control beads that were not treated with any dye will stay in Q4 (Cy5 -, MBBR -). These populations are gated based on the fluorescence intensity of control compound **3**.



Section-9A: Fluorescence readout of 64 scaffolds after cyclization.







K1-[AAA]: Incomplete cyclization was detected on 10 μm but was >90% complete on 160 μm beads.







K2-[ABA]: Complete cyclization was observed on 10 μ m & 160 μ m beads.






K3-[ACA]: Incomplete cyclization was observed on both 10 μ m and 160 μ m beads.















K7-[AAB]: Incomplete cyclization was observed on 10 μ m but was complete on 160 μ m beads.







K8-[ABB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.







K9-[ACB]: Incomplete cyclization was observed on both 10 μ m & 160 μ m.









K10-[ADB]: Incomplete cyclization was observed on both 10 μ m & 160 μ m beads.







L1-[BAA]: Cyclization was incomplete on 10 μ m beads but was complete on 160 μ m beads.







L2-[BBA]: Complete cyclization was observed on 10 μm & 160 μm beads.







L3-[BCA]: Cyclization was complete on both 10 μ m & 160 μ m beads.













L7-[BAB]: Complete cyclization was observed on 10 µm & 160 µm beads have >90% cyclization complete.









L8-[BBB]: Complete cyclization was observed on 10 µm & 160 µm beads.







L9-[BCB]: Complete cyclization was observed on 10 µm & 160 µm beads. A linear (2.5mer) fragment could not cyclize (MW 1478, RT- 8.124). Other fragments (2.5mers) cyclized and identified.








L10-[BDB]: Complete cyclization was detected on 10 μ m but was incomplete on 160 μ m.









M1-[CAA]: Complete cyclization was observed on 10 µm & 160 µm beads.







M2-[CBA]: Complete cyclization was observed on 10 μ m & 160 μ m beads.







M3-[CCA]: Complete cyclization was observed on 10 μ m & 160 μ m beads.







M4-[CDA]: Complete cyclization was observed on both 10 μ m & 160 μ m beads.







M7-[CAB]: Complete cyclization was detected on 10 μ m but was incomplete on 160 μ m beads.









M8-[CBB]: Complete cyclization was observed on 10 μm but 160 μm had incomplete cyclization.









M9-[CCB]: Incomplete cyclization was observed on both 10 μm and 160 μm beads.









M10-[CDB]: Complete cyclization was observed on 10 μm but 160 μm beads had incomplete cyclization. Linear precursor was detected (MW 1674, RT- 8.40).









N1-[DAA]: Complete cyclization was observed on 10 μ m &160 μ m beads.



100





N2-[DBA]: Complete cyclization was observed on 10 μ m &160 μ m beads.







N3-[DCA]: Complete cyclization was observed on 10 μ m &160 μ m beads.







N4-[DDA]: Complete cyclization was observed on 10 μ m &160 μ m beads.







N7-[DAB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.






N8-[DBB]: Complete cyclization was detected on 10 µm but was incomplete on 160 µm beads.







N9-[DCB]: Incomplete cyclization on both 10 μm and 160 μm beads, linear starting material was identified in small quantity (MW 1674, RT 8.376).







N10-[DDB]: Cyclization was complete on both 10 µm & 160 µm beads.





O1-[AAD]: Incomplete cyclization was detected on 10 µm but was complete on 160 µm beads.





O2-[ABD]: Cyclization was complete on both 10 μ m & 160 μ m.







O3-[ACD]: Incomplete cyclization was detected on 10 µm but was complete on 160 µm beads.







O4-[ADD]: Cyclization was complete on both 10 μ m & 160 μ m beads.







O7-[AAC]: Cyclization was complete on both 10 μ m & 160 μ m beads.







O8-[ABC]: Cyclization was complete on both 10 μ m & 160 μ m beads.







O9-[ACC]: Cyclization was complete on both 10 μ m & 160 μ m beads.











P1-[BAD]: Cyclization was complete on both 10 μ m & 160 μ m beads.







P2-[BBD]: Cyclization was complete on both 10 μm & 160 μm beads.







P3-[BCD]: Cyclization was complete on both 10 μ m & 160 μ m beads.







P4-[BDD]: Cyclization was complete on both 10 μ m & 160 μ m beads.






P7-[BAC]: Cyclization was complete on both 10 μ m & 160 μ m beads.













P9-[BCC]: Cyclization was complete on both 10 μ m & 160 μ m beads.







P10-[BDC]: Incomplete cyclization was detected on 10 μm but was complete on 160 μm beads.







Q1-[CAD]: Cyclization was complete on both 10 μ m & 160 μ m beads.







Q2-[CBD]: Cyclization was complete on both 10 μ m & 160 μ m beads.







Q3-[CCD]: Cyclization was complete on both 10 μ m & 160 μ m beads.









Q4-[CDD]: Cyclization was complete on both 10 μ m & 160 μ m beads.







Q7-[CAC]: Incomplete cyclization was detected on 10 μ m but completed >90% on 160 μ m. A linear fragment (3.0-mer, MW 1593) were detected.









Q8-[CBC]: Cyclization was complete on both 10um & 160um. Dead beads could be due to 1.5mer linear fragments (MW 1300).













Q10-[CDC]: Incomplete cyclization was detected on 10um but was complete on 160um.









R1-[DAD]: Cyclization was complete on both 10um & 160um.



R2-[DBD]: Cyclization was complete on both 10um & 160um.






R3-[DCD]: Cyclization was complete on both 10um & 160um.







R4-[DDD]: Cyclization was complete on both 10um & 160um.





R7-[DAC]: Cyclization was complete on both 10um & 160um.







R8-[DBC]: Cyclization was complete on both 10um & 160um.







R9-[DCC]: Cyclization was complete on both 10um & 160um.







R10-[DDC]: Cyclization was complete on both 10um & 160um.





Amines (ŷ L CH **V** \bigcirc \mathcal{Q} £ Ľ H_JN 1,N~ R R Jo € O € C -L H₂N \mathcal{O} H₂N s s 1 ¢ ↓ ↓ ↓ Ł L. s s ~~~ HAN , ↓ · · i. L. s s H₂N₄ H₂N₄ H₂N₄ K € CH iy, s and the second ۰ţ H,N~~~N~N HO P Br NH₂ H₂N N C Ň H₂N N H₂N HO H₂N H₂N N HO_O s H₂N < Contraction of the second se H_JN H₀N 1 HO C R H₂N H₂N~~ N H₂N H₂N N •^I он Стран HO CO H₂N~O , O HAN CO HO O S HN QX of the HO O S HO_FO_R HO_FO_R CI i (j H_eN NH₂ H_JN NA CAN < ↓ CH CH H_IN £ HOLO H₂N~~_O H₂N N s s °¹r× HU LO H,N C H_NM H,N N HO O S H₂N N HO S ic H.N. 5 ₩^Ĺ NH₂ но R R но H₂N₄ H₃N₄ K NH₂ но H₂N NH, HAN H,N s s H,N H₂N , i O L. H_NN H₂N - Car L CH ∩ CH 6 r H₂N₄ H₂N₄ H₂N₄ R s s ° H₂N \bigcirc H₂N • م **∕**µ

Section-9: Sequencing result of beads separated by flow cytometer due to incomplete cyclization (upto 3 copies)

30	MolecularID 130224031502281017022804 6	H _k N~0		ACCC (A) 3 miles AVIIIINES (A2)	Amines (U2) states Adds (U2)	ADDS (K2) SINKS AND ADD (K2)	NCC1=CC=CO1	Acids (03) smiles CICC1=CC(C(0)=O)=CC=C1
31	130224031503280217102804 6	H _I N	NCCCOC HOLLOCI	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=C(S(=O)(C)=O)C=C1	00(C1=C0C(CC()=N1)=0 H ₂ N	NC8@H(C/C1=CC=C1.(S)	0=C(0)C1=C(C)0C=C1
40	130424031502281017032809 6	H ₂ N~0	HOLDOC HOLDOC			encicle:cle884(incic)=o		ocilof84(c)c0=of81
60	130224101509280217032801 5			CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1		NCCC1=ONC2+CC=CC+C21	OC([C(gH](C)C()=O[S]
61	130224101510280117092804 5			CICC1=CC(C(0)=0)=CC=C1			N(CQH)(C)C1=CC=CC=C1 (R)	ODC(0)=0
74	131024031502280217092803 5	H _N N		OC(C1=CSC(CG(HN1)=0		00(01=000(00()=N1)=0	N(C@H)(c)c1=Cc=Cc1 [R] HOOO	oci[c@H](c)c(=0.[5]
48	130124071501280617032803 5	NH ₂		OC(C1=COC(CC)=N1)=O		0C(C1=CC=C(CC)C=C1)=0	NCCCNIC+ON+C1 HO_O	0C([C(gH](C)C()=0.[S]
49	130124071501280917032809 5	NH ₂		00(C1=C00(C0)=N1)=0	NCC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(CCI)=N1)=0	HOUDOCCI HOUDO	oc([c@H](c)c(=o.[s]
50	130124071503280417092804 5	NH ₂		00(C1=C0C(CCI)=N1)=0		00(C1+CC+C(C0)C=C1)=0 H_101_00	N(C@H)(C)C1=CC+CC=C1 [R]	000(0)=0
51	130124071510280417092804 5	NH ₂	NCC1=CC=C(C)C=C1	00(C1=C00(CCI)=N1)=0		CICIC(C)=C(C@8H((C)C(O)=O	N(C@H)(C)C1=CC=CC1 (R)	CCC(0)=0
57	130224071502280717022803 5	NH ₂	NCC1=CC=C(C)C=C1	CICC1=CC(C(O)=O)=CC=C1		00C(C1=CS0(CC1)=N1)=0	HOCCNIC=CN=C1	CICC1=CC(C(0)=O)=CC=C1
58	130224071504280317032803 5		NCC1=CC=C(C)C=C1	CICC1=CC(C(O)=O)=CC=C1	NCC1=CC=CS1	00C(C1=COC(CC()=N1)=0	HOUDONIC=CN=C1	oci[c@H](c)ci=o [S]
59	130224071510290317032804 5	NH ₂	HO HO CI	CICC1=CC(C(0)=0)=CC=C1		CCCIC(c)=C(C@BH(C)C(0)=0	HO_O	CCI[C@H](C)CI=O [S]
65	130324071501290217042804 5	NH ₂	NCC1=CC=C(C)C=C1	00(C1+C5C(CC()+N1)=0	NCC1=CC=C(S(=O)(C)=O)C=C1	00(C1+C0C(CC()+N1)=0	NCC1=CC=CO1 HO_O R	OC([C@H](C)8r)=O.[R]
66	130324071501280417042803 5	S NH2	NCC1=CC=C(C)C=C1	00(C1=C5C(C0)=N1)=0		00(C1=CC=C(CC) C=C1)=0	NCCCN1C=CN=C1 HO_O R	0C([C@H](C)Br)=0.[R]
70	130424071501280417032809 5	NH ₂	HO HO			00(C1=CC=C(0C0)C=C1)=0	HOUDOCCI HOUDO S	oci[C@Hi(C)Ci=O[S]
46	130124051509280417032805 5	H ₂ N	NCC1=CC=G(0CC2)C2=C1		NCC1=CC=CC(C(F)(F)F)=C1	ccc/c)+c/c98H(c/c/o)+o	NCC1000(0+C0+C2)=0201 H0_0 S	oci[c@H(c)c)=o[s]
47	130124051510280417032801 5	H ₁ N	NCC1=CC=G(0CC2)C2=C1	00(C1+C00(C0)+N1)+O			NCCC1=CNC2+CC=CC=C21 HO_O S	oci[c@H[(c)c)+O[s]
63	130324051501280217022803 5	H ₂ N ⁻	NCC1=CC=C(0CC2)C2=C1	OC(C1+CSC(CC()+N1)=0	NCC1+CC+C(S(+O))C)=0)C=C1	00(C1=COC(CC()+N1)=0	NCCCNIC+CN+C1	CICC1=CC(C(0)=O)=CC=C1
64	130324051502280817092803 5	H ₁ N	NCC1=CC=G(0CC2)C2=C1	OC(C1=CSC(CC(I=N1)=O		00(C1=CC=C(CC)(C=C1)=0 H_2N=C	N(C@H)(c)c1+cc+cc+c1 (R)	oci[c@H(c)c)=o.[s]
71	130924031509280417012803 5	H ₁ N	NCCC1CCCCC1	OC(C1=CSC(CC(I=N1)=O	NCC1=CC=CC(C(F)(F)F)=C1		NCCONIC=ON=CI	OC(C1=CSC(CCI)=N1)=O
72	130924031509290417032810 5	H ₂ N	NCCC1CCCCC1	00(C1=C5C(CC)+H1)=0	NCC1=CC=CC(C(F)(F)F)=C1		NCCC1=CC=C(OC)C(OC)=C1 HO_O CI S	oci[C@+](C)C)=O[S]
73	130924041504280417032806 5	H ₂ N				00(C1=CC=0(0CI)C=C1)=0	NC(CQH)(C)C1=CC=CC=C1	0C([C@H](C)C(=0.[S]
52	130224031501260417032806 5	H ₂ N~~o~	HOTCI	CICC1=CC(C(0)=0)=CC=C1		00(C1=CC=C(CG)C=C1)=0	NC(C@H)(C)C1=CC+CC=C1	oci[c@H(c)c)=o.[s]
53	130224031501280817032803 5	H ₂ N~~0	HO HO CI	CICC1=CC(C(0)=0)=CC=C1	N(CQQH)(C)C1=CC=CC=C1	00(C1=C3C(CCI)=N1)=0		0C([C@H](C)C(=0.[S]
ñ4	130224031501281012042803 5	H _I N~~0~	HO LOCAL					ocilo@Hi(c)Ri=o [R]
66	130224031501281017092804 6	H _I N~~0	HO HO CI	CICC1=CC(C(0)=0)=CC=C1			NC(BH)(c)c1=cc=cc1[R]	000(0)=0
66	130224031503281017032803 6	H _M N~~~~	NCCCOC HU LI	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=C(C)C=C1	cicic(c)=c/c@@H(ic)c(c)=o	NCCCNTC=DN=C1	oc([c@H(c)c(=o.[s]
62	130324031502280817092803 6	H _I N~~_O	NCCCOC	OC(C1=CSC(CD(=N1)=0		ocict=csc(oci)=N1)=O	NC(2H)(C)C1=CC=CC1 [R]	ocilc@Hi(c)ci=otal
67	130424031501280317032809 6	H _A N~~_O	HO HO CI	cicic(c)=ci(c@@H)(c)c(o)=0		ocict=cocicc(i=N1)=0	HOUSE S	ocilc@Hi(c)ci=otal
60	130424031002280417042806 6	H _k N~~o~						00((0)(0)(C)(Br)=0.[R]
	130224101001300417032808 5	H _i N						ocilo@nicoci+o[S]
114	130424101001200017032803 4	HN		HIN THE				00/108/10/00-0.[8]
116	130424101009200017032803 4	HN						college source
115	130424101508250417032503 4	HN		H ^N U L		H'N N		ocio@eiccenoisi
107	120224081602280317012803 4	HN		H ₂ N Y				
70	130124071601380347922904 4	HN		H ₂ N Y		H ₂ N C		001108HILC/01=0.[S]
*0	100124071001280317032804 4			H ₂ N Y				001000100010010015
00	100124071001280817032806 4	NH ₂				HILLES CONTRACTOR		outogrif(C)CI+O.[S]
01	130124071502280817032803 4			NH,		H2N N		ocijugelj(C)Ci=O.(S)
82	130124071503280217102803 4	NH ₂	NUU1=00=0(0)0=01	H_N 0	NUU1=CC=0(S(=0)(C)=0)(C=C1	UU(U1=COC(CC()=N1)=0	NU-12800+0(C/C1=DC=CC=C1.[S] H0_0 S	oc([c@H(c)ct=o(s)
83	130124071504280817032806 4	NH ₂				unicial contraction HPM	HOUTUDO(C=CC=C2)=C2O1	ocic@Hi(c)ci=o.[s]

84 130124071510280317012803 4	NH2 NCCI=C	xx=c(c)c=c1	, NH2		HJN		OC(C1=CSC(CCI)=N1)=O
91 130224071502280417032805 4	NCC1=C	xx=c(c)c=c1 HOTCTTCI	H ₂ N N O		HAN	NCC1C00(C=CC=C2)=C2O1	ocijc@Hj(c)ci=o(s) S
9/2 13022/40/150328001/022804 4	NCC18C		HAR YOX		H ₂ N	HO HO	
93 130224071503281017042803 4	NCC1=C	XX=C(C)C=C1 H0 C(C)C=C(C(0)=0)=CC=C1	HĮN		H,N	NCCCN1C=CN=C1 HOO	OC([C@H](C)Br)=O.[R]
94 130224071504280417042803 4	NCC1=C	C=C(C)C=C1	H _N N H _N O			HOUSE HOUSE	OC([C@H](C)Br)=O.[R] R
85 130224071509260217042809 4	NH2 NCC1=C	CCC(G)C=C1	HAN		H ₂ N	HOLO	OC([C@H](C)8r)=O.[R] R
104 130324071501280317032803 4	NCC1=C	xx=c(c)c=c1	H _E N	NCC1=CC+CS1	H ₂ N	NCCCN1C=CN+C1	oci[C@H[(c)ci=o.[8]
106 130324071501280717032803 4	NH2 NCC1=C	xx=c(c)/c=c1	- NH,	N0C1=CC=D(NC)C)C=C1	HJN	NCCCNIC=CN=C1	ocilc@Hi(c)ci=o.(s)
108 130324071503281017032803 4	NCC1+C	xx=c(c)c=c1	H ₂ N		H ₂ N N	NCCCN1C=CN+C1	S
78 130124051502280917032803 4	H ₁ N O	x==c(occ2;c2=c1	ward X	NDC1=CC(F)=CC(C(F)(F)=C1	H ₂ N	NCCCN1C=DN=C1	oci[C@H[(C)C)=0.[S]
100 130324051501280917032803 4	H ₂ N OCT=C	xx=c(occ2;c2=c1	wardly,	NCC1=CC(F)+CC(C(F)(F)F)=C1	H ₂ N N	NCCCN1C=CN+C1	ocijc@Hj(c)ci=o[S]
101 130324051502280317032805 4	HIN NCCIEC	xx=c(occ2;c2=c1	H ^I N.	NCC1=CC+CS1	HAN	NCC1C0C(C=CC=C2)=C2O1	OCI[C@H](C)CI)=O [S]
102 130324051502280417032804 4	H ₂ N CC1=C	xx=c(occ2;c2=c1	H ₂ N N O		H _N N	NCC1=CC=CO1	oci[C@H](C)Cl)=O [S]
103 130324051504280417032802 4	H ₂ N CC1=C		H _J N N O		H _I N	NCCO HOLO	0C([C@H](C)C()=0.[S] S
112 130424051502280717042810 4	H _k N CC1=C		A NH		HANCOL	NCCC1=CC=C(OC)C(OC)=C1	BrC1=CC=C(C(0)=0)C=C1
113 130424051503280717032803 4	H ₁ N OCT=C				Hin		ocijc@Hi(cici)=o.(s) S
75 130124011503280317032803 4	H ₂ N Br NCC1+C		H ₂ N		H ₂ N N	NCCCNIC=CN+C1	ocijc@Hj(c)ci)=o.[S] S
77 130124041502280817032803 4	NCC=C		2		H ₂ N	NCCCNTC=CN+C1	oci[C@H[(C)C)=O.[S]
116 130624021502280817032804 4	H ₂ N		2		H ₂ N	NCC1=CC+CO1	oci[C@H[(C)C)=0.[S] S
117 130924021502280817092803 4	H,N NCCC10		2		H ₂ N R	N(C@H)(C)C1=CC=CC1 [R]	oci[C@H[(C)C)=O.[S]
118 130624031503280817032802 4	H _J N		2		н _и м ОН	NCCO HOLO	ccic@Hickci+o.[s]
119 130824031503280817032808 4	H ₂ N NCCC1C		2		HJN	NCC1CCOCC1	0C [C@H](C)C)=0.[S]
120 130624031504260317032810 4	H ₂ N NCCC1C		H ₂ N			NCCC1=CC=C(OC)G(OC)=C1	oc([C@H[(C)C)=0.[S]
121 130924031509280117032810 4	H _J N		HAN			NCCC1=CC=C(0C)C(0C)=C1	oci[c@H[(c)c)=o.[3] S
122 130824031509280317092804 4	H,N NCCC1C		HAN		H _A N R	N(C@H)(C)C1=CC=CC=C1 (R)	CCC(0)=0
123 120624031510200217032804 4	H ₂ N		NH2		H ₂ N		ocijc@Hicicieo(s) S
76 130124031502280717032810 4	H _N N~~_O					NCCC1=CC=C(OC)G(OC)=C1	ocijc@Hi(c)ci=o.(s) S
86 130224031501260917022809 4	H ^I N~~~~		NN COX	NOC1=CC(F)=CC(C(F)(F)F)=C1	H _a N	NCC1CCOCC1	CICC1=CC(C(0)=0)=CC=C1
87 130224031501251017102804 4	H _k N~~_O	C C C C C C C C C C C C C C C C C C C	H ₂ N		H ₂ N ₄ s	N(C@@H((C)C1=CC=CC=C1.[5]	0=0(0)01=0(0)00=01
88 130224031502261017032803 4	H _I N~NCCCOO	C C C C C C C C C C C C C C C C C C C	H ₂ N		H ₂ N N	NCCCNTC=CN=C1	oci[c@H[(c)c)=o.[s]
89 130224031503260717032804 4	H _N N~NCCCOO	C HO C C C C C C C C C C C C C C C C C C	A NH		H _L N	NCC1=CC=CO1	ocijc@Hj(c)ci=o.[s] S
90 130224031503280917032803 4	H ₂ N~~_O	C C CC1+CC(C(0)=0)=CC+C1	which the second	NCC1+CC(F)+CC(C(F)(F)F)+C1	HJN	NCCCNTC=CN+C1	oci[C@H[(c)c)=o.[S]
97 130324031001200517032509 4	H _N N~~_O		2		Han	NECTICCOCCT HOLO	oci[c@H(c)c)-o.(8]
98 130324031503280917102804 4	H _k N~O		na contra	NOC1=CC(F)=CC(C(F)(F)F)=C1	H ₂ N S	N(C@@H)(C)C1=CC=CC=C1.[5]	0=0(0)01=0(0)00=01
99 130324031504280817022809 4	H _i N^^O		2		H _N	NCC1CCOCC1	~C
108 130424031503280217092804 4	H _k N~~_O		HAN	NCC1=CC=C(S(=O)(C)=O)C=C1	H ₂ N R	N(C@H)(C)C1=CC=CC=C1 (R)	CCC(0)=0
100 130424031509280417092803 4	H _A N~O	c corc(c)=c(c@@H)(c)c(o)=o	HAN		H ₂ N F R	N(C@H)(C)C1=CC=CC=C1 (R)	oci[c@Hj(c)ci=0.[8]
110 130424031610280417032807 4	H_N O				~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=00(00)=00(00)=01	ocijc@Hj(c;ci=o.(s) S
111 130424031510280417092803 4	H ₂ N O NCCCOO		LNH.		H ₂ N ₂ R	N(CBH)(C)C1=CC=CC=C1 [R] HO O	ocilc@Hitcictr=o.[s]
157 130124101501280317032803 3			H ₂ N	NCC1=CC+CS1	H ₂ N N		0C([C@H](C)C(=0.[S] S
191 130224101503280417102803 3			H _M N		H ₂ N ₄ S	NC80H(C)C1=CC=CC=C1.[5] H0 0	ocilc@Hi(C)C(=0.[5]
192 130224101504280317012803 3		2N1 CICC1=CC(C(0)=0)=CC=C1	H2N	OH OC(1=000)(C(1=000)(C(0+H1)=0) NOC1=0000(C(1=000)(C(0+H1)=0) 000000000000000000000000000000000000	H ₂ N N		OC(C1=CSC(CCI)=N1)=O

Enter	MolecularID Conjur Aminor (VI	Aminge (V1) emilier Acide (V1)	Acide O(1) emilee Aminee (V2)	Aminor OCD emilar Acids OCD	Acids OCD emilar Aminos (V2)	Aminor OCII emilor Acide OCII	Acide OCD emiles
193	130224101504280017092804 3 HN		CICC1=CC(C(0)=0)=CC=C1	NCC1=CC(F)=CC(C(F)(F)F)=C1	OC(C1=CSO(OCI)=N1)=O	N(CQH)(C)C1=CC=CC1 (R)	CCC(0)=0
194	130224101508280217032807 3 HIV		CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1		NCC1=CC(OC)=CC(OC)=C1	OCI[C@H](C)CI=O [S]
195	1302241015102802170902803 3 HN				000(0)=0(08884)(00(0)=0 H_2N_2 R		ocilo@viloici=o.(s)
238	130424101504280017032800 3 HN			NCC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(CC()=N1)=0	NCC1CCOCC1 HOO	0C [C@H](C)Cl)=0 [S]
190	130224081504280717032803 3 HN		CICC1=CC(C(0)=0)=CC=C1		00(01=CSD(C0)=N1)=0	NCCCNIC=CN=C1 HO_O S	0C([C@H](C)C()=0.[S]
263	131024031603280817032803 3 H ₂ N		OC(C1=CSC(CCI)=N1)=0		00(C1=CSO(OCI)=N1)=0	NCCCNIC=CN=C1 HO S	OCI[C@H](C)CI=O.[S]
254	131024031504280017032803 3 H ₂ N	F NCC1=CC(F)=C(F)C=C1	OC(C1=CSC(CC)=N1)=0	NOC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(CC)=N1)=0	NCCCNIC=CN+C1 H0_0 5	0C([C@H[(C)CI)=O.[S]
135	130124071501280217032807 3	NH2 NCC1=CC=C(C)C=C1	OC(C1=C0D(0CI)=N1)=0	NCC1=CC=C(S(=0)(C)=0)C=C1	0C(C1=COC(CC()=N1)=0	NCC1=0C(0C)=CC(0C)=C1 H0 0 5	oci[C@H[(C)CI)=0.[5]
138	130124071501280317032809 3	NH ₂ NCC1=CC=C(C)C=C1	0 0C(C1+C0C(CCI)=N1)=0 H ₂ N J ⁵		0C(C1=COC(CC()+N1)=0	NCC10C00C1 H0_0 5	0C([C@H[(C)CI)+O.[S]
137	130124071501280817102804 3	NCC1=CC=G(C)C=C1	0C(C1=C0C(CCI)=N1)=0	N(c@@H)(c)c1=cc=cc=c1	00(01=CSO(00)=N1)=0 H ₂ N	N(C@@H(C)C1=CC=CC1(S) OH	0=C(0)C1=C(C)0C=C1
138	130124071502280117102804 3	NH2 NCC1=CC=C(C)C=C1	OC(C1=COC(OCI)=N1)=O H ₂ N/~O		0C(C1=COC(CC()=N1)=0 H ₂ N	N(C@@H)(C)C1=CC=CC=C1 [S]	0=C(0)C1=C(C)0C=C1
139	130124071502280217102803 3	NH2 NCC1=CC=C(C)C=C1	0C(C1=C0C(CC)=N1)=0	NCC1=CC=C(S(=O)(C)=O)C=C1	0C(C1=COC(CCI)=N1)=0 H ₁ N	N(C@@H)(C)C1=CC=CC=C1.[5] H0_0 5	0C([C@H](C)C(=0.{S]
140	130124071502280317012809 3	NH ₂ NCC1=CC=C(c)C=C1	0 0C(C1=C0C(CCI)=N1)=0 H ₂ N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CS1	0C(C1=COC(CCI)=N1)=0	NCC10C00C01	OC(C1=CSC(CCI)=N1)=O
141	130124071502280417042807 3	NH2 NCC1=CC=C(C)C=C1	0C(C1=C0C(CC)=N1)=0 H		00(01=00+0(00)(0=01)=0	NCC1=CC(OC)=CC(OC)=C1 HO _ O R	0C([C@H](C)Br)=0.[R]
142	130124071502280817082804 3	NH2 NCC1=CC=C(C)C=C1	OC(C1=C0C(CCI)=N1)=0		00(01=00=0(00)(0=01)=0 H_2N=0 R	N(C(gH)(C)C1=CC=CC=C1 (R)	CCC(0)=0
143	130124071502280917032807 3	NH2 NCC1=CC=G(C)C=C1	OC(C1=COC(CCI)=N1)=O	NOC1=CC(F)=GC(C(F)(F)F)=C1		NCC1=CC(OC)=CC(OC)=C1 HOOO 5	OCI[C@H](C)CI=O.[S]
144	130124071502281017032810 3	NH ₂ NCC1=CC=G(G)C=C1	0C(C1=C0C(CCI)=N1)=0			NCCC1=CC=C(0C)C(0C)=C1 H0 5	0C([C@H[(C)CI)+O [S]
145	130124071503280417102802 3	NH2 NCC1=CC=G(C)C=C1	0C(C1=C0C(CCI)=N1)=0 H ₂ N	NCCNC(C)=0	00(01+00+0(00)0+01)+0 H_N	NC88H(C/C1+CC+CC+C1 [S] HO	CICC1=CC(C(O)=O)=CC=C1
148	130124071503280917032804 3	NH2 NCC1=CC=G(G)C=C1	0C(C1+C0C(CCI)=N1)=0	NGC1+CC(F)+GC(C(F)(F)F)+C1	00(01+CSQ(00)+N1)+0	NCC1=CC=CO1 HO O 5	0C([C@H[(C)CI)+O [S]
147	130124071504280417032809 3	NH ₂ NCC1=CC=C(C)C=C1	CC(C1=COC(CCI)=N1)+O		0C(C1=CC+C(CC)(C=C1)=0	NCC10C00CC1 HO	oci[c@H[(c)ct+o.[s]
148	130124071504280517102803 3	NH2 NCC1=CC=G(C)C=C1	OC(C1=COC(CCI)=N1)=0		00(01=00=0(00)0=01)=0 H_2N	NCB@H(C/C1+CC+CC+C1.[5] H0	0C([C@H[(C)CI)+O [S]
149	130124071504280817032804 3	NH ₂ NCC1=CC=C(C)C=C1		Мовенисосто	00(01=050(00)=N1)=0	NCC1=CC+CO1 HOO	OCI[C@H](C)CI+O[S]
150	1301240715042800917032803 3	NH ₂ NCC1=DC=C(C)C=C1	0C(C1=C0C(CCI)=N1)=0	NCC1=CC(F)=CC(C(F)(F)F)=C1	00(01=CS0(00)=N1)=0	NCCCNIC=CN=C1	oci[c@H[(c)ci)=0.[s]
151	130124071504280917032806 3	NH ₂ Noct=cc+c(c)c=c1		NCC1+CC(F)+CC(C(F)(F)F)+C1	00(01=050(00)=N1)=0	NC(c@H)(c)c1+cC+cC+C1 HO	oci[c@H[icici+o.[s]
152	130124071509280117092803 3	NH ₂ NCC1=CC=C(C)C=C1		NCC1=CC=CC(C(F)(F))F)=C1	CIC/C(C)=C(C@@H)(C)C(O)=O	N(CQH)(C)C1=CC=CC=C1 (R)	OC([C@H](C)CI)=O.[S]
153	130124071508280217012803 3	NH2 Nontencer(r)rent					00(01=050(00)=N1)=0
154	3	NH ₂ NCC1=CC=C(C)C=C1			CIC/C(c)=C(C000H(C)C(O)=O	N(C@@H(C)C1=CC=C1[5]	0=C(0)C1=C(C)0C=C1
155	1301240715102800317022804 3	NH ₂ NCC1=CC=C(C)C=C1	OC(C1=COC(CCI)=N1)=O	CC(C)CCN			CICC1=CC(C(O)=O)=CC=C1
171	130224071501280417092803 3	NH ₂ NCC1=CC=C(C)C=C1	CKC1=CC(C(0)=0)=CC=C1		0C(C1=CC=C(CC)(C=C1)=0	N(C@H)(C)C1=CC=CC=C1 [R] H0 5	oci[c@H[(c)ci)=o.[s]
172	130224071501280717012803 3	NH ₂ NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1		0C(C1=CSC(0CI)=N1)=0		OC(C1=CSC(CCI)=N1)=O
173	130224071501280717032802 3	NH ₂ NC1=CC=C(C)C=C1	CICC1=CC(C(O)=O)=CC=C1		00(01=050(001)=N1)=0 H ₂ N	HOLO HOLO S	oci[c@H[(c)ct=o.[s]
174	130224071501280817042809 3	NH ₂ NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1	Моженисоста	0C(C1=CSC(CCI)=N1)=0	HOLOGOOCT	OC([C@H](C)Br)=O.[R]
175	3	NH ₂ NG1-cc-c(c)c-c1	CICC1-CC(C(0)-0)-CC-C1		co(c)-cc-o(co)(c-c))-o	NEC1-52(00)-00(00)-01	oc([c@H](c)c)-o.[a]
176	3	NH ₂ NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1		00(01=CC=0(00)(C=01)=0	NCCCNIC=CN=C1	0C([C@H](C)CI=0.[S]
177	3	NH, NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1		00(01=CC=0(00)(C=01)=0	NCCCNIC=CN=C1	oc([C@H](C)CI=0.[S]
178	130224071504280317102804 3	NH ₂ NCC1=CC=G(C)C=C1	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CS1	00(01=000(00()=H1)=0 H3/H 5 5	NC@@H(C/C1=0C=CC1[S]	0=C(0)C1=C(C)0C=C1
179	130224071504280517032803 3	NH ₂ NCC1=CC=Q(C)C=C1	CICC1=CC(C(0)=0)=CC=C1		0C(C1=CC=C(CCI)C=C1)=0	HOCCNIC=DN=CI	oc([c@H](c)ct)=0.[S]
180	130224071504280717012803 3	NH ₂ NC01=CC=G(C)C=C1	CICC1=CC(C(0)=0)=CC=C1		00(01=050(001)=N1)=0		OC(C1=CSC(CCI)=N1)=O
181	3	NH ₂ NCC1=CC=G(G)C=C1	CICC1=CC(C(0)=0)=CC+C1			NCCCNIC+CN+C1 HO	oci[c@H[(c)ch+o.[s]
182	3	NH ₂ NCC1=CC=C(C)C=C1	H_N	NCC1=CC=CC(C(F)(F)F)=C1		NCCCNIC=ON=C1 HO	0C([C@H](C)CI)=0.[S]
183	3	NH ₂ NCC1=CC=G(C)C=C1	H_N + ++++++++++++++++++++++++++++++++++	NOC1=CC=CC(C(F)(F)F)=C1		HO ¹ HO ¹ HO ¹	CICC1=CC(C(O)=O)=CC=C1
184	3	NH ₂ NCC1+CC+C(C)C+C1	H_N + ++++++++++++++++++++++++++++++++++	HOCT+CC=CC(C(F)(F)F)=C1	acc(c)=C[C@@H](C)C(0)=O	HOUDOUCCI HOUDO S	ocijc@Hj(c)ctr+o.(sj

enuy	The copies Printes (c)	Phillips (Cr) strikes (Cr)	Autor (A) Sinks Autor (A2)	Pullika (va) allika Pulla (va)	Autor (ks)	700 LB (C) SILLES 700 LB (C)	70005 (CO) STILLES
185 130	22240715002800317032810 3	NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1		NCCC1=CC=C(OC)C(OC)=C1	OCI[CBH](C)CI=O[S]
186 130	224071509260417032802 3	NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1	CICIC(C)=C(C@@H)(C)C(O)=O	NCCO HOUGO S	OC([C@H](C)C)=O.[S]
187 130	2240/1510/24011/10/2404 3		CCC1=CC(C(0)=0)=CC=C1		and check and ch		0=0(0)01=0(0)00=01
188 130	224071510280217102804 3	NCC1=CC=C(C)C=C1	CICC1=CC(C(0)=0)=CC=C1	HO HO CI	CICIC(C)=C[C@@H](C)C(O)=O	N(C@@H)(C)C1=CC=CC1.[S]	0=C(0)C1=C(C)0C=C1
189 130	224071510280317042807 3	HOTOCICCICCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	CICC1=CC(C(0)=0)=CC=C1	CC(C)CCN HO		NCC1=CC(0C)=CC(0C)=C1	0C([C@H](C)Br)=0.[R]
207 130	324071501260217042803 3		OC(C1=CSC(CC()=N1)=0	NCC1=CC=C(S(=0))C)=0(C=C1	0C(C1=COC(CC()=N1)=0	NCCCNIC=ON=C1 HO	OC([C@H](C)Br)=O.[R]
208 130	324071501280217102804 3	NCC1=CC=C(C)C=C1	0C(C1=CSC(CC()=N1)=0	NCC1=CC=C(S(=0)(C)=0)C=C1	00(01=000(00()=N1)=0	NC@@H(C)C1=CC=CC=C1 [S]	0=C(0)C1=C(C)0C=C1
209 130	324071501260317032808 3		0C(C1=CSC(CCI)=N1)=0		00(01=000(00(I=N1)=0	Brc1=CC=D(CN)C=C1	oc([c@H](c)c(=0.[5]
210 130	324071501260417032803 3		OC(C1=CSC(CC(=N1)=0		0C(C1=CC=C(CC)C=C1)=0	NCCCNIC=CN+C1 HO	0C([C@H](C)C)=0.[S]
211 130	324071503280817032809 3	NCC1=CC=C(C)C=C1	OC(C1=CSC(CC()=N1)=O	N(C@@H)(C)C1=CC=CC=C1	00(C1=CSO(CCI)=N1)=0	NCC1CCOCC1 HOLO	OC([C@H](C)C()=O.[S]
212 130	324071503281017092803 3		OC(C1=CSC(CCI)=N1)=O		CIC/C(c)=C(C@@H)(C)C(0)=0 H_2N=K	N(C@H)(C)C1=CC=CC1 (R)	OC([C@H](C)C()=0.[S]
213 130	324071504280417042801 3	NCC1=CC=C(C)C=C1	0C(C1=CSC(CCI)+N1)=0	NCCNC(C)=0	00(01=00=0(00)0=01)=0	NCCC1=CNC2=CC=CC=C21	OC([C@H](C)Br)=O.[R]
214 130	324071510200317032808 3		0C(C1=CSC(CC)+N1)=0			BrC1=CC=D(CN)C=C1	OC([C@H](C)CI)=O[S]
232 130	424071501200817032803 3	NCC1=CC=C(C)C=C1	CIC(C)=C(C33H)(C)C(0)=0	N 088H)(c)c1=cc=cc=c1	00(C1=CSO(0C1)=N1)=0 H ₁ N N	NCCCNIC=CN=C1 HO_O 5	OC([C@H](C)C)=O[S]
233 130	424071504200617102804 3	NCC1=CC=C(C)C=C1	CIC(C)=C(C@@H)(C)C(0)=0	NCC1=CC=CC=C1 0+	00(01=00=0(00)(0=01)=0 H_2/H_2/H_2 5		0=C(0)C1=C(C)0C=C1
234 130	424071509290017012803 3		CIC/C(C)=CI(C@@H)(C)C(O)=O	NCC1=CC=CC(C(F)(F)F)=C1			OC(C1=CSC(CCI)=N1)=O
235 130	424071500280417002804 3		CICIC(C)=C(C\$\$\$H)(C)(O)=0	NCC1=CC+CC(C(F)(F)F)=C1	CICIC(C)=C(C@@H(C)C(O)+O H_2N=C R	N(CBH)(c)c1=CC=CC=C1 [R]	CCC(0)=0
128 130	124051501280817042804 3 H ₂ N	NCC1=CC+C(OCO2)C2+C1	OC(C1=COC(CCI)=N1)+O	NCC1+CC+CC+C1	0C(C1=CC+C(CC)C=C1)+0	NCC1=CC+CO1 HO	0C([C@H](C)8r)=0.[R]
129 130	124051501280817042808 3 H ₂ N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		OC(C1=COC(CCI)=N1)=O		0C(C1=CC+C(CC)C=C1)+0 H ₂ N	BrC1+CC+Q(CN)C+C1	0C([C@H](C)8r)=0.[R]
130 130	124051503260917032803 3 H ₂ N	NCC1=CC=C(OCO2)C2=C1	0C(C1=C0C(CC)=N1)=0	NCC1=CC(F)+CC(C(F)(F)F)+C1	00((C1=CSC(CC1)=N1)=0	NCCCNTC+ON+C1 HO_O	0C([C@H](C)C(HO [S]
131 130	124051504280417022809 3 H ₂ N	NCC1=CC=C(OCO2)C2=C1			0C(C1=CC+C(CC)(C=C1)=0		CICC1=CC(C(O)=O)=CC=C1
132 130	124051508280217032807 3 H _J N	NCC1=CC=C(0CC2)C2=C1		NCC1=CC=CC(C(F)(F)F)=C1		NCC1=CC(OC)=CC(OC)=C1	OCI[C@H](C)CI=O [S]
133 130	124051508280317022806 3 H ₂ N	NCC1=CC=C(OCO2)C2=C1		NOC1=CC=CC(C(F)(F)F)=C1		NC(C@HQ(C)C1=CC=CC1	CICC1=CC(C(0)=0)=CC=C1
134 130	124051510260417022806 3 H _J N	NCC1=CC=C(0CC2)C2=C1				NC(C@H)(C)(C1=CC+CC+C1	CICC1=CC(C(0)=O)=CC=C1
168 130	224051501280817092803 3 H _J N	NCC1=CC=C(OCO2)C2=C1	CICC1=CC(C(0)=0)=CC=C1	N(D@@H)(C)C1=CC=CC=C1	0C(C1=CS0(CCI)=N1)=0 High R	N(C@H)(C)C1=CC=CC1 (R) H0 0 5	0C([C@H](C)C(=0.[S]
168 130	224051002300717033004 3 H ₂ N + ++++++++++++++++++++++++++++++++++					HODISOCION HOUSE	ocile@Hitcict=o.(s)
170 130	224051504200917042804 3 H ₂ N	HO HO CI	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC(F)=CC(C(F)(F)(F)=C1	0C(C1=CSC(0CI)=N1)=0	NCC1=CC=CO1	OC([C@H](C)Br)=O.[R]
197 130	324051501260617032806 3 H ₂ N	NCC1=CC=C(OCC2);C2=C1	OC(C1=CSC(GC()=N1)=O NH2	NCC1=CC=CC=C1	0C(C1=CC=C(CC)(C=C1)=0	NCC1C0C(C=CC=C2)=C2O1 H0 0 5	oci[c@H[(c)ci=o.[s]
198 130	324051501280917032809 3 H ₂ N	NCC1=0C=C(0CC02)C2=C1	0C(C1=CSC(CC()=N1)=0	NCC1=CC(F)=CC(C(F)(F)(F)=C1	0C(C1=CSO(0CI)=N1)=0	HOUTOCOCCI	oc([C@H](C)ci=o.[s]
199 130	324051502280717032804 3 H ₃ N	NCC1=0C=C(0CC2)C2=C1	OC(C1=CSC(CC(=N1)=0	NCC1=CC=C(N(C)C)C=C1	0C(C1=CSC(0CI)=N1)=0	NCC1=0C=CO1 HOLO	oc([C@H](C)ci=o.[s]
200 130	324051502261017032803 3 H ₂ N	NCC1=OC=C(OCO2)C2=C1	OC(C1=CSC(CC)=N1)=0	HOC1=CC=C(CI)C=C1	cicricia=cice@@Hitcicicia=c	NCCGNIC=ON=C1 HO_O S	oc([c@H](c)ct=0.[5]
201 130	324051503260317032803 3 H ₃ N	NCC1=CC=C(0CC2)C2=C1	CC(C1=CSC(CC)+N1)=0	NCC1=CC=CS1	0C(C1=COC(CC1)+N1)=0	NCCCNIC=CN=C1 HO_O S	OC([C@H](C)C)=O.[S]
202 130	324001003200717032610 5 H ₃ N	NEC1-CC-C(0C02)C2-C1	CC(C1-CSC(CCI)-N1)-0		oc(c1-cac(ccl)-N1)-o	NECCI-CC-C(OC)C(OC)-C1	oc(lo@H(c)c)-o.(a)
203 130	324051504260917022809 3 H ₃ N	NCC1=DC=C(OCC2)C2=C1	0C(C1=C5C(CCI)=N1)=0	NDC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(0CI)=N1)=0	HO HO CICCOCCI	CICC1=CC(C(O)=O)=CC=C1
204 130	324051509290217032801 3 H ₃ N	NCC1=DC=C(0CC2)C2=C1	OC(C1=CSC(CCI)=N1)=0	NDC1=CC=CC(C(F)(F)F)=C1		NCCC1=CNC2=CC=C21	OC([C@H](C)C(=0.[S]
205 130	324051509260217042803 3 H ₃ N	NCC1=DC=C(OCO2)C2=C1	OC(C1=CSC(CCI)=N1)=0	NDC1=CC=CC(C(F)(F)F)=C1		NCCCNIC=ON=C1 HO	OC([C@H](C)Br)=0.[R]
206 130	324051510260417032805 3 H ₃ N	NCC1=0C=C(0C02)C2=C1	OC(C1=CSC(CCI)=N1)=0	HO HO CI		NCC1COC(C=CC=C2)=C2O1	oc([C@H](C)C(=0.[S]
228 130	3 H ₂ N + + + + + + + + + + + + + + + + + + +				00(01=050(001)=N1)=0	NCCC1=CNC2=CC=CC1	ocilc@H(c)ci=o.(s)
229 130	424051502260717032803 3 H ₂ N	NCC1=CC+C(OCC2)C2=C1	CCCC(C)=C(C3(3(H))(C)C(0)=0			HOUSE S	ocilc@H(c)ci+o.(s)
230 130	424051504200317102801 3 H ₃ N	NCC1=CC=C(OCC02)C2=C1			0C(C1=CSC(CCI)=N1)=0 H,JN	N(C@@H)(C)(C1=CC=C1.[S]	OC(C1=CSC(CC1=N1)=O
231 130	3 H ₂ N + + + + + + + + + + + + + + + + + + +		CICIC(C)=C(C@@H)(C)C(0)=0	NDC1=CC(F)=CC(C(F)(F)F)=C1		NCC1000(0=CC=02)=0201	00([C@H](C)C(=0.[S]
124 130	124011502260917032809 3 H_N/TC+Br	NCC1=OC=CC(Br)=C1	0C(C1=C0C(CC)=N1)=0	NCC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(CCI)=N1)=0	HOUTOCOCCI	ocilc@Hi(c)ct=o.[5]

Entry 239	130924021504260917032803 3	Amines (X1) smiles Acids (X1)	Acids (K1) smiles Amines (X2) CICC1#CCIC/Oi#Oi#C0#C1	Amines (Q) smiles Acids (Q)	Acids (02) smiles Amines (X3)	Amines (03) smiles Acids (03) NCCCN1CuCNuC1	Acids (03) smiles
	H ₂ N	ното	HAR CAL		HJN	HO O S	estate de la
240	130924031501280617042804 3 H.N	NCCC1CCOCC1	OC(C1=CSC(CC)=N1)=0	NCC1=CC=CC=C1	00C(C1=CC=C(CCI)C=C1)=0	NCC1=0C=CO1 HO R	OC([C@H[(C)8r)=0.[R]
241	13092403150128031/012803 3					NCCCNTC=CN=CT	OC(C1=CSC(CC)=N1)=O
242	130624031502280317032804 3	ИСССТССОССТ УТСТ		NCC1=CC=CS1		NCC1=CC=CO1 HO O	oci[c@H[(c)ct)=0 [S]
243	130824031502280317032808 3	NCCC10COCC1	OC(C1=CSC(CC(=N1)=0		00(C1=COC(CC()=N1)=0	Brc1=CC=C(CN)C=C1	OC([C@H](C)C()=O.[S]
244	130624031502280617012803 3		OC(C1=CSC(CC(=N1)=0		00(C1=CC=C(CC)C=C1)=0 H ₂ N///N/N/N		OC(C1=CSC(CCI)=N1)=O
245	130624031502280817042808 3		OC(C1=CSC(CC()=N1)=O		0C(C1+CC+C(CC)C+C1)+0 H2N	BrC1=CC=C(CN)C=C1	OC([C@H](C)Br)=O.[R]
246	130924031502280817012809 3					NCC1CCOCC1	OC(C1=CSO(CCI)=N1)=O
247	H,N 130624031502281017012800 3		CC(C1=CSC(CC()=N1)=0				0C(C1=CSC(CCI)=N1)=0
248	130624031504260817032806 3						0C([C@H](C)C)=0.[S]
249	H ₂ N 130624031508280117012809 3	NCCC1CCCCC1	OC(C1=CSC(CC()=N1)=0	NCC1=CC=CC(C(F)(F)F)=C1		NCC10C00CC1	OC(C1=CSC(CCI)=N1)=O
250	H ₂ N 130624031508280117022805 3		00(C1=C5C(CCI)+N1)=0	HO CI		NCC1COD(C=CC=C2)=C2O1	CICC1=CC(C(O)=O)=CC=C1
251	HJN HJN	NCCC1CCCCC1	H_N	H0 + CI		H0 ⁴ () N(C8@H)(C)C1=CC=CC=C1 [S] ()	0=C(0)C1=C(C)0C=C1
252	H _J N	NCCC10COCC1					CICC1=CC(C(0)=O)=CC=C1
	H _J N ⁻			HOTICI	H ₂ N	нотора	00/07/10/01-07/2
130	H ₂ N		R, R T T		H ₂ N C	HO S	ociognicici-o(s)
236	130424091504280717032806 3 H ₂ N		CICIC(C)=C(C@@H)(C)C(0)=0	NCC1=CC=C(NC)C)C=C1	DOC(C1=CSO(CCI)=N1)=O	NCC1COD(C=CC=C2)=C2O1	oci[c@Hi(c)ci=o.(s)
237	130424091506280317022803 3 H ₂ N		H2N + ++++++++++++++++++++++++++++++++++	NCC1=CC=CC(C(F)(F)F)=C1	cicic(c)+c/c@@HI(c)c(o)+0		CICC1=CC(C(O)=O)=CC=C1
125	130124031502280717032808 3 H _N N	NCCCOOC	00(C1+C00(C0)+N1)+0			NC(C@H)(C)C1=CO+CC=C1	OCI[C@H](C)CI+O.[S]
128	130124031502280917012809 3 H ₂ N~~O	NCCCOC			DC(C1=CSC(CCI)=N1)=O	NCC1CCOCC1	OC(C1=CSC(CCI)=N1)=O
127	130124031510280417032804 3 H_N	NCCCOC	00(C1=C0C(C0)=N1)=0			NCC1+CC+CO1 HO S	ocijc@Hj(c)cti+0.[S]
158	130224031502280817032804 3 H _e N~~~~~		CICC1=CC(C(0)=0)=CC+C1		00(C1+CC+C(CC)C+C1)+O	H0_0 s	oci[c@H[(C)CI)=O.[S]
159	130224031502280717032809 3 H ₂ N~~O~	NCCCOC NOT CI	CICC1=CC(C(0)=0)=CC=C1		DC(C1=CSC(CCI)=N1)=O	NCC10C00CC1 HO O S	OC([C@H](C)Cl)+O [S]
160	130224031502281017032806 3 H_N	NCCCOC HOLY CI	CICC1=CC(C(0)=0)=CC=C1			NCC1COD(C=CC=G2)=G2O1	OC([C@H](C)C()=O.[S]
161	130224031503280317032803 3	NCCCOC HOLICI	CICC1=CC(C(0)=0)=CC=C1				ocilc@Hi(c)ch=o.[s]
162	130224031503280817032804 3	NCCCOC	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC=C1	0C(C1=CC=C(CC1)=0 H ₂ N	NCC1=CC=CO1 HO O	0C([C@H](C)Cl=0.[S]
163	130224031504280917102804 3						0=0(0)(01=0(0)00=01
164	130224031508280217102804 3	NCCCOC		NCC1=CC=CC(C(F)(F)F)=C1			0=C(0)C1=C(C)0C=C1
165	130224031508280417082804 3	NCCCOC P		H0 CI		N(C@H)(C)C1=CC=CC=C1 [R]	CCC(0)=0
166	130224031508280417102804 3	NCCCOC P		NCC1=CC=CC(C(F)(F)F)=C1		ViceBeHildCoteccectite] / OH	0=D(0)C1=D(C)0C=C1
167	130224031510280117092804 3	HO CI	H_NF		CICHO(C)=C/(CØØH(C)C(O)=O H,N	N(C@H)(C)C1=CC=CC=C1[R]	CCC(O)=0
196	H ₂ N 0	HO HO C	OC(C1=CSC(CC()=N1)=0		00(C1=CC=C(CC1)=O	NCCCNIC=CN=C1 HOO	0C([C@H](C)8r)=0.[R]
215	H ₂ N~~_O~	NCCCOC				NCCO R	OCIT/CIRHITCICI+O (SI
	HAN	но	RIN TOX		H ₂ N OH	HOLO S	eele® iteree e tel
210	H_N 0		His Ch			How S	ociotaticicio (s)
217	130424031502280217032802 3			NCC1=CC=C(S(=O)(C)=O)C=C1	H ₁ N OH	HO S	oc([c@H](c)c)=o.(s]
218	130424031502280817032803 3	HO HO			00(C1=CSC(CCI)=N1)=0	NCCCNIC=ON=C1 HO	oc([c@H](c)c(=0.[S]
219	130424031503280817032806 3 H ₂ N~~O~	HO HO CI			DC(C1=CSC(CCI)=N1)=0	NCC1000(C=CC=C2)=C201	oc([c@H](c)ct)=0.[S]
220	130424031503280017032803 3 H ₂ N~~O	NCCCOC HOLE C	CICIC(C)=C(C@@H)(C)C(O)=O	NDC1=CC(F)=CC(C(F)(F)F)=C1	DC(C1=CSC(CC1)=N1)=0	NCCCNIC=CN=C1 HO S	0C([C@H](C)Cl=0.[S]
221	150424031503280917102803 3 Hj.N	NCCCOC HOLES	CICIC(C)=C(C@(2H)(C)C(0)=0	NCC1=CC(F)=CC(C(F),F)F)=C1	00(C1=CSC(CCI)=N1)=0 H,N	N(C@@H(IC)C1=0C=CC=C1 [S] HO O S	OC(]C@H](C)C()=O.[S]
222	130424031504280317012803 3 H ₂ N	NCCCOC	CICIC(C)=C(C3(2)H)(C)C(0)=0	NCC1+CC=CS1	00(C1=C0C(CC0+N1)=0		0C(C1=CSC(CCI)=N1)=O
223	130424031504290817032809 3 H ₂ N~~~O~	NCCCOC		N(CB(BH)(C)C1=CC=CC=C1	DC(C1=CSC(CC()=N1)=0		0C([C@H](C)C(=0.{S]
224	130424031506260217022803 3 H.N	NCCOOC	CICICIC)=C(C002H)(C)C(0)=0	NCC1=CC=CC(C(F)(F)F)=C1			CICC1=CC(C(O)=O)=CC=C1
225	130424031509280217032810 3	NCCCOC					OCI[C@H[(C)CI)=O.[S]
	n ₂ n - 0	HOTA	· · · · · · · · · · · · · · · · · · ·	HOTA	HAN	, a	

228	MolecularID Co 130424031509290417032802 3	pies Amines (X1)	Acids (X1) Acids (X1) Acids (X1) smiles NCCCOC CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	Amines (82)	Adds (x2) Adds (x2) <t< th=""><th>Attines (X3)</th><th>Amines (G) smiles Acids (G) NCCO HO₂ _ O</th><th>OC([C(gH](C)Cl)=O.[S]</th></t<>	Attines (X3)	Amines (G) smiles Acids (G) NCCO HO ₂ _ O	OC([C(gH](C)Cl)=O.[S]
		H ₂ N	HO	HAN	но	H ₂ N OH	s s	
227	130424031510280317032802 3	H_N		L م		H,N OH	HO O	OC([C@H](C)C()=O.[S]
332	130124101501280/1/032803 2	un		V NH2			NCCONTCHONECT HO_O	ocilo@elicicieo.[s]
		NH	с с ^{са}	NH2	а С ^л	H ₂ N UN	×a s	
333	130124101504280917032803 2	HN		HAN CON	NCC1=CO(F)=CO(G)=V(G)(F)=F)=C1	H ₂ N N	HO S	oc([c@H((c)c)=0.[s]
427	130224101501280217022806 2	HN	C1CNCCN1 CH CICC1=CC(C(0)=0)=CC=C1	H_N	NCC1=CC=C(8(=0)(C)=0)(C=C1	0		CICC1=CC(C(0)=0)=CC=C1
428	130224101501281017022809 2	ŃH	C1CNCCN1 Q CKC1=CC(C(0)=0)=CC=C1	~~~		NH ₂		CICC1=CC(C(0)=O)=CC=C1
		HN	HOTOCI	HAN CO	HO	H ₂ N ^r	но	
429	130224101501281017032808 2	HN		HAN		H _k N	Brc1=cc=c(cN)c=c1	OCI[CigH](C)CI)=O[S]
430	130224101502260517032802 2	HIV		OH CH	NCC(C)(C)O	→ OH	NCCO HO O	0C([C@H](C)C()=0.[S]
431	130224101502290617012803 2	NH	HO [*] U [*] C C1CNCCN1 0 CICC1=CC(C(0)=0)=CC=C1	nja 🔨	NCC1=CC=CC=C1 00(C1=CC=C)(C01C=C1)=0	H'N.		OC(C1=CSC(CCI)=N1)=O
		HN	HOTO	NH ₂		H ₂ N N N	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	
432	130224101502280817032803 2	HN		Q	N(CBGH)(C)C1=CC=CC=C1	H ₂ N	NCCCN1C=CN=C1 HO S	OC([C@H](C)C()=O.[S]
433	130224101502280817032808 2	HN	C1CNCCN1 CICC1=CC(C(0)=0)=CC=C1		N(08@H)(0)C1=CC=CC=C1 ОС(С1=CSC(CC()=N1)=O	HIN	BrC1=CC=C(CN)C=C1 HO_O	OC([C@H](C)Cl)=O.[S]
434	130224101503280817032802 2	NH NH		, Kang	NICERENCICI=CC=CC=C1	Br	NCCO	OCIC/RHI/CICI=O/SI
		HN	HO TO TO			H ₂ N	s s	
435	130224101504280517092804 2	HN		H _L N	NCC(C)(C)0 0C(C1=CC=C(CC)(C=C1)=0	H ₂ N	N(C@H)(C)C1=CC=CC=C1 (R)	CCC(O)=0
438	130224101504280817042810 2	HN	C1GNCGN1 C1CC1=CC(C(0)=0)=CC=C1	Ó			NCCC1=CC=C(OC)C(OC)=C1 0	BrC1=CC=C(C(0)=0)C=C1
617	1202241016022804 2	NH		X.		H _M	HO	001084101010181
517		HN		NH ₂		H ₂ N	HO COULD S	00108/10/01/02/01
556	130424101501280517102804 2	HN		NH ₂		Hall	NCB@H(IC)C1=CC=CC=C1.[5]	0=C(0)C1=C(C)0C=C1
567	130424101501280917032809 2	HN		NACK		H,N	NCC1CCOCC1 H0_0	0C([C@H](C)CI)=O[S]
558	130424101501280817082803 2	, NH		Ŷ		HANNER	NC2HV0C1+CC+CC+C1/R1	OCICRHICICI+O ISI
		HN	но	NA CAL		6 ª	s s	
559	130424101502280317092803 2	HN		H ₂ N	NCC1+CC=CS1	H _i N _i R _R	N(c@H)(c)c1+cc+cc+c1.(R) H0 5	OC([C@H](C)C()=O[S]
560	130424101503280717032807 2	HN		4.0			NCC1=CC(0C)=CC(0C)=C1	0C([C@H](C)C()=0.[S]
561	130424101503260917012803 2	NH		NH,	NCC1=CC(F)=CC(C(F)(F)F)=C1 (C(C)=CC(CC)=N1)=O	X		0C(C1=CSC(CCI)=N1)=O
		HN	HU A A A A A A A A A A A A A A A A A A A	N/N CCC		H ₂ N		
562	130424101504280817092804 2	HN		Q	N(C88H)(C)C1=CC=CC=C1	H _A N _K R	N(C@H)(C)C1=CC=CC=C1 (R)	CCC(O)=0
663	130424101509260417032807 2	HN			NCC1=CC=CC(C(F)(F)F)=C1		NCC1=CC(0C)=CC(0C)=C1 H0 0	0C([C@H](C)C(=0.[S]
584	130424101510280417012804 2	ŃH				X	NCC1=CC=CO1	OC(C1=CSC(CCI)=N1)=O
		HN	HO	NH ₂	HO	H ₂ N		
327	130124051501280917102503 2	HN		NA CAR	NCC1=C0(F)=CC(0(F)(F)F)=C1	HUN S	N(c@@H)(c/c1=cc=cc=c1.(8)	oc([c@H](c)c)=0.[s]
378	130124081602280317032803 2	HN		H ₂ N		H,N NNN		00([08)4](0)00(5)
329	130124081502260517102804 2	NH H	NICGNCCC1 CC(C1=00C(Cd)=N1)=0	ОН		нда	N(C@@H)(C)C1=CC=CC=C1.[5]	0=C(0)C1=C(C)0C=C1
220	12012/00/00/2020/12022/00/	NH		HĨN. X	он с с с	0 5		001000100-0101
		HN	L .	A CANH		H,N O	HO S	
331	130124081504280817032803 2	HN		9	N(C@@H)(0)C1=CC=CC=C1	H,N NN	HO S	OC([C@H](C)C()=O.[S]
420	130224081501280717032801 2	HN			NCC1=CC=D(N(C)C)C=C1	0	NCCC1=CNC2=CC=CC=C21 HO_O	0C([C@H](C)C()=0[5]
421	130224081504260717102803 2	- MH	HO CI CI CI CI =CC(C(0)=0)=CC=C1	NH ₂	NCC1=CC=D(NC)C/C=C1 /	H,N	No@@H(c)c1=cc=cc=c1.(s)	0C([C@H](C)C(=0.[S]
		HN	HOTCI	NH,		6 s	s s	
511	130324081503280817032803 2	HN		NH ₂		H _J N N	NCCCN1C+CN+C1 HO S	OC([C@H](C)C()=O.[S]
012	130324051504280417042808 Z	HN			ИССИСІС-0 ОД СП ОСІСІ-СС-СІССІС-СІ)-0	H ₂ N	BrC1-CC-C(CN)C-C1 HO O	oc([cgH](c)8)-o.[4]
613	130324081504280617042804 2	NH	NICCNCCC1		N0C1=CC=CC=C1	Br	NCC1=CC=CO1 HO. +O	0C([C@H](C)8r)=0.[R]
		HN	∼ K u	C NH,	CH CH	H ₂ N	R	
514	130324081504280717032802 2	HN		4	NCC1=CC=C(N(C)C)C=C1	H ₂ N	NCCO HOUD S	oc([cgH](c)c(=0.[S]
647	130424081508280217042803 2	HN		H,N Y		H ₂ N N		0C([C@H](C)Br)=0.[R]
618	131024031502280617092803 2	H _N N Y	NCC1=CC(F)=C(F)C=C1			HJN	N(C(gH))C)C1=CC=CC=C1 (R) HOO	0C([C@H](C)C()=0.[S]
	12102102100	4		U NH2		O R	S S	001000
919	131024031504280717032804 2	H ₂ N		A NH		H ₂ N	HOUT-DEREUT	Ju([ugp4](C)C(=0.[S]
620	131024031504280817022803 2	HAN		Q .		H ₂ N~NN		CICC1=CC(C(0)=0)=CC=C1
621	131024031509280417012803 2	H _N N	NCC1=CC(F)=C(F)<	NH,	OC OH NCC1=CC=CC(C(F)(F)F)=C1 OCC(C)=C1[C@@H](C)C(O)=O			OC(C1=CSC(CCI)=N1)=O
283	130124071601280317022806	Y		HAN		-12/10 IV		0001=000000000000
	2	NH ₂		H ₂ N			Herton	
284	130124071501280317032808 2	NH ₂	NCC1+CC+C(C)C+C1	H ₂ N		Ŷ	NC(C@H)(C)C1+CC+CC+C1 HO_O	0C([C@H](C)C)=0[S]
			CH		ОН	NH2		

285	130124071501280617032801 2	copies runnes (cr)	NCC1=CC=C(C)C=C1	OCICI-COCICI-N1WO	NOCLECCECCEC	00/01#00#01/#0	NOCC1#CNC2#CC#CC#C21	OC/IC/RHI/C/C/#O [S]
		NH ₂		NH ₂			HO S	eele@.itoiso e.tel
286	130124071501280717032801 2	NH ₂	NCC1=CC=C(C)C=C1	OC(C1=COD(CCI)=N1)=0	NCC1=CC=C(N(C)C)C=C1	0C(C1=CSC(CCI)=N1)=0	NCCC1=CNC2=CC=CC21 HO S	OCI[C@H](C)CI)=O.[S]
28/	1301240/1501280/1/102803 2	NH ₂						ocilo@vi(c)ci=o(si
288	130124071501280817012803 2	NH ₂	NCC1=CC=C(C)C=C1		N(C@@H)(C)C1=CC=CC=C1	00(C1=CS0(CCI)=N1)=0 H ₂ N		OC(C1=CSC(CCI)=N1)=O
289	130124071501280817092804 2		NCC1=DC=C(C)C=C1	OC(C1=COD(CCI)=N1)=0	N(CQ)QH)(C)C1=CC=CC=C1	00(C1=CSC(0CI)=N1)=0 H3/N	N(CQH)(C)C1=CC=CC=C1 (R)	CDD(0)=0
290	130124071501280917032801 2		NCC1=CC=C(C)C=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1		NCCC1=CNC2=CC=CC21 H0 0	OC([C@H](C)C()=O.[S]
291	130124071501290917042804 2		NCC1=CC=C(C)C=C1	000(C1=C000(C0)=N1)=0	NCC1=CC(F)=CC(C(F)(F)F)=C1		NCC1=CC+CO1 H0_0	OC([C@H](C)8r)=0.[R]
292	130124071501281017032808 2		NCC1=DC=C(C)C=C1				BrC1=CC=D(CN)C=C1	0C([C@H](C)C(=0.[S]
293	130124071502280217032801 2				H0 H0 NCC1=CC=C(S(=0)(C)=0)C=C1		NCCC1=CNC2+CC+CC+C21 H0 - 0	0C([C@H](C)C)=0.[S]
294	130124071502280217032808 2	NH ₂					NCICAHICICI-CC=CC=C1	OC/IC@HI/C/CI=O/ISI
000	1001010710000011000010	NH ₂				MH ₂	× s	0010011000100101
190	130124071502200317032810	NH ₂		H ₂ N	Nuclicicus	H _M N	HO S	ocijognicici)=o.(sj
296	130124071502280417032801 2		NCC1=CC=C(C)C=C1		NCCNC(C)=0	0C(C1=CC=C(CC))C=C1)=O	NCCC1=CNC2=CC=CC21	OCI[C@H](C)CI)=O.[S]
297	130124071502280417042802 2	NH ₂	NCC1=CC=C(C)C=C1	0C(C1=C0C(CC)=N1)=0	NCCNC(C)=0	oc(c1=cc=c(cc);c=c1)=0	NCCO HOUSE R	OC([C(BH](C)Br)=O.[R]
298	130124071502290517092803 2	NH ₂	NCC1=CC=C(C)C=C1	OC(C1=COC(CCI)=N1)=O H ₂ N		0C(C1=CC=C(CC)C=C1)=0 H_2N=C	N(C@H)(C)C1=CC=CC=C1 (R)	OCI[C@H](C)CI=O.[S]
299	130124071502280717032802 2	NH ₂		OC(C1=COD(C0)=N1)=0		00(c1=cS0(00)=N1)=0	NCCO HO S	OC([C@H](C)C()=O.[S]
300	130124071502280817042809 2	NH ₂	NCC1=CC=C(G)G=C1			00(C1=CS0(0C1=N1)=0	NCC10C00CC1 HO R	OC([C@H](C)Br)=O.[R]
301	130124071502280917022809 2	NH ₂	NCC1=CC=C(C)C=C1	00(C1=C00(CCI)=N1)=0	NCC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(CCI)=N1)=O		CICC1=CC(C(O)=O)=CC=C1
302	130124071502281017022805 2			OC(C1+COC(CCI)=N1)+O			NCC1C00(C+CC+C2)+C201	CICC1=CC(C(O)=O)=CC=C1
303	130124071503280317032801 2		NCC1=CC+C(C)C+C1			0C(C1=COC(CC()+N1)=0	NCCC1=CNC2+CC=CC=C21	0C([C@H](C)CI)=O.[S]
304	130124071503280317032803 2		NCC1=CC=C(C)C=C1	0C(C1=C0C(CCI)=N1)=0				0CI[C@H](C)CI=0 [S]
305	130124071503280417042804 2					0C(C1=CC=C(CC)(C=C1)=0	NCC1=CC+CO1 HO O	OC([C@H](C)8r)=O.[R]
306	130124071503280817032804 2						NCC1=CC+CO1 HO O	0C([C@H](C)C)=0 [S]
307	130124071503280917032803 2		NCC1=DC=C(C)C=C1	OC(C1=COC(C0)=N1)=O	NCC1=CC(F)=CC(C(F)(F)F)=C1	00(01=CS0(001=N1)=0		0C([C@H](C)C()=0.[S]
308	130124071503280917042803 2				NCC1=CC(F)=CC(C(F)(F)(F)=C1			OC([C@H](C)Br)=O.[R]
309	130124071503280917092804 2		NCC1=CC=C(C)C=C1		NCC1=CC(F)=CC(C(F)(F)F)=C1	00(01=CS0(00)=N1)=0 HJ/N	N(CQH)(C)C1=CC=CC=C1 (R)	CCC(0)=0
310	130124071804280217032805 2							nc(ng)4(n)n(m) (s)
311	130124071504280317032801 2		NCC1=CC=C(C)C=C1			0C(C1=COC(CC()+N1)=0	NCCC1=CNC2=CC=CC1 H0. 40	oc(ic@Hi(c)c(=o.[s]
312	130124071604260317032806 2	J NH2					NCC20HICCC1=CC=CC1	OC/IC/MHI/C/C/=0.1SI
313	120124071504280417022803 2	NH ₂		H ₁ N				0001-0000-00-00-01
515	130124071004200417022803	NH ₂	Contracticities and the second s	H ₂ N N Y		H _J N N	HOTOT	0001-00(0(0)-0)-00-01
314	130124071504280417032801 2	NH ₂	NULTIECCEC(C)CEC1	H,N N H			HOLUI=CNC2=CC=C21	uci[C@H[(C)C(=0.[S]
315	130124071504280417032803 2	NH ₂	NCC1=CC=C(C)C=C1	HIN HO		00(c1=cc=c(ccl(c=c1)=0	NCCCNIC=ONECI HOUS	ocilc@Hi(c)ci=o [s]
316	130124071504280417032808 2	NH ₂	NCC1=CC=C(C)C=C1	HzN N O		0C(C1=CC=C(CC)C=C1)=0	Br01=CC=C(CN)C=C1	0C([C@H[(C)C)=0 [S]
317	130124071004200417042800 2	NH ₂	NCC1-CC-C(C)C-C1	oc(c1-COC(CCI)-N1)-0	HCCHC(C)-0	00(01-00-0(00)(0-01)-0		oc([c@H](C)Br)-o.[4]
318	130124071504280617032806 2	NH ₂	NCC1=CC=C(C)C=C1	OC(C1=COD(C0)=N1)=O	NCC1=CC=CC=C1	00(C1=CC=D(CCI)C=C1)=0	NCC1000(C=CC=C2)=C201	0C([C@H(C)C(=0.[S]
319	130124071504280917012808 2	NH,	NCC1=CC=C(C)C=C1	0C(C1=C0C(CC)=N1)=0	NCC1=C0(F)=C0(C(F),F)F)=C1	0C(C1=CSC(CCI)=N1)=0 H ₂ N	Brc1=CC=C(CN)C=C1	OC(C1=CSC(CCI)=N1)=O
320	130124071509280117012804 2	NH ₂	NCC1=CC=C(C)C=C1	OC(C1=COC(CCI)=N1)=O	NCC1=CC=CC(C(F)(F)F)=C1		NCC1=DC=CO1	OC(C1=CSC(CCI)=N1)=O
321	130124071509280217032801 2	NH ₂	NCC1=0C=C(C)C=C1		NCC1=CC=CC(C(F)(F)F)=C1		NCC01=CN02=CC=C21	0C([C@H](C)C(=0.[S]
322	130124071509280217032802 2	NH ₂	NCC1=CC=C(C)C=C1				NCCO HOLO S	0C([C@H](C)C(=0 [S]
323	130124071509280317012809 2		NCC1=CC=C(C)C=C1		NCC1=CC=CC(C(F)(F)F)=C1			0C(C1=CSC(CC)=N1)=0
324	130124071509280317042809 2							0C([C@H](C)8r)=0.[R]
325	130124071509280417092801 2		NCC1=CC=C(C)C=C1		HO T CI		NC@H()C)C1=CC=CC1 [R]	OC(C1=CSC(CCI)=N1)=O
328	130124071510280417022805 2		NCC1=CC=C(C)C=C1				NCC1000(C=CC=C2)=C201	CICC1=CC(C(0)=O)=CC=C1
		,	→ A	NH ₂	HOTA		HOTO	

Section-11: Analysis of Naive bead population: These beads are deep sequenced after DEL synthesis

Entry 1	Molecular ID 130424081501260117032808	Copies 47	Amines (X1)	Amines (X1)- smiles N1CCNCCC1	Acids-(X1)	Acids-(X1) smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines-(X2)	Amines-(X2) smiles NCCOC	Acids-(X2)	Acids-(X2) smiles OC(C1=COC(CCI)=N1)=O	Amines-(X3)	Amines-(X3) smiles BrC1=CC=C(CN)C=C1	Acids-(X3)	Acids-(X3) smiles OC([C@H](C)CI)=O.[S]
			HN		HOLING		H ₂ N O		o= CH		H ₂ N		HO O S	
2	130124071501260717022810	44	NH ₂	NCC1=CC=C(C)C=C1	OCI	OC(C1=COC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1	CI CI CH	OC(C1=CSC(CCl)=N1)=O	***~~Q	NCCC1=CC=C(OC)C(OC)=C1	но	CICC1=CC(C(0)=0)=CC=C1
4	130224101503260317102804	37	HN	CICNCCNI		CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1-CC-CS1	CI C	OC(C1=COC(CCI)=N1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[8]	OH O	O=C(O)C1=C(C)OC=C1
3	130224031504260517032802	37	H ₂ N~~o~	NCCCOC	" ¹ 0~	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O	\mathcal{L}	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N~~OH	NCCO	HO S	0C([C@H](C)Cl)=0.[S]
5	130324041504260417092804	33	MH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	H _I N~ ^H +°	NCCNC(C)=O	\sim	OC(C1=CC=C(CCl)C=C1)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
6	130424071502260917032805	31	NH ₂	NCC1=CC=C(C)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H,N	NCC1COC(C=CC=C2)=C2O1	HO S	0C([C@H](C)Cl)=0.[S]
7	130424061502260517032802	25	H ₂ N	NCC1=CC=CO1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
8	131024021502261017022809	23	HIN TO	NCC1=CC(F)=C(F)C=C1	но	CICC1=CC(C(O)=O)=CC=C1	H,M	NCC1=CC=C(Cl)C=C1	·	CIC/C(C)=C/[C@@H](C)C(O)=O	HĮN	NCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1
9	130224091509260317032803	19	1.1 ~ <u>~</u>	NCCCN1C=CN=C1	носто	CICC1=CC(C(O)=O)=CC=C1	HAN Y	NCC1=CC=CC(C(F)(F)F)=C1	···l	CIC/C(C)=C/[C@@H](C)C(O)=O	"" "	NCCCN1C=CN=C1	HO S	ОС([C@H](C)Cl)=О.[S]
11	130924031509260217102804	18	н,м	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	-lpipo	CIC/C(C)=C/[C微復H](C)C(O)=O	H,N 5 .	N[C@@H](C)C1=CC=CC=C1.[S]	0 OH	0=C(0)C1=C(C)0C=C1
10	130124041509260317022804	18	///NH2	NCC=C		OC(C1=COC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CC(C(F)(F)F)=C1	·	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	" ¹ O"	CICC1=CC(C(O)=O)=CC=C1
12	130124071501260417102804	17		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H _I N	NCCNC(C)=O	J. J	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S]	0 OH	O=C(O)C1=C(C)OC=C1
13	130224031503260417092804	16	H _I N~~o~	NCCCOC	новоро	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCCNC(C)=O	\sim	OC(C1=CC=C(CCI)C=C1)=O	H,N	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	0=000000
14	131024021501260417102804	16	H ₂ N ¹	NCC1=CC(F)=C(F)C=C1	HO ^L CO ^{CO}	CICC1=CC(C(O)=O)=CC=C1	H _N N	NCCNC(C)=O	~_C^~	OC(C1=CC=C(CCI)C=C1)=O	H _N N	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
15	130124061509260117102804	15	H ₂ N	NCC1=CC=CO1		OC(C1=COC(CCI)=N1)=O	NAN Y	NCC1=CC=CC(C(F)(F)F)=C1	···lpipo	CIC/C(C)=C/[C微微H](C)C(O)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S]	0 OH	O=C(O)C1=C(C)OC=C1
16	130124071510260417032803	15	NH ₂	NCC1-CC-C(C)C-C1	O=OH	OC(C1-COC(CCI)-N1)-O		CC(C)CCN		CIC/C(C)-C/[C@@H](C)C(O)-O	**~~Q	NCCCN1C-CN-C1	HO O S	0C([C@H](C)CI)=0.[8]
17	130124101510260317092804	14	HN	CICNCCNI		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	"lpin	CIC/C(C)=C/[C@@H](C)C(O)=O	H _I N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
18	130224101510260317032803	14	HN	C1CNCCN1	нојото	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	··· leri	CIC/C(C)=C/[C@@H](C)C(O)=O	"	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
19	130224021501260417042806	13	H ₂ N	NCC1=CC=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCCNC(C)=O	Salar and the second se	OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O R	OC([C@H](C)Br)=O.[R]
23	130224031510260417092804	12	H ₂ N~~0~	NCCCOC	HOLOGI	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	·· h	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=0
22	130124081504260417102804	12		N1CCNCCC1	O OH	OC(C1=COC(CCI)=N1)=0	H,N H	NCCNC(C)=O	\mathcal{L}	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	0=C(0)C1=C(C)0C=C1
26	130424031510260317032803	12	H _I N O	NCCCOC	HOLY	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	··· lpi	CIC/C(C)=C/[C@\@H](C)C(O)=O	**~~~~ ~ \}	NCCCN1C=CN=C1	HU U S	0C([C@H](C)Cl)=0.[S]
21	130124081502261017042803	12		N1CCNCCC1	O= OH	OC(C1=COC(CCI)=N1)=0	H,M	NCC1-CC-C(CI)C-C1	- lan	CIC/C(C)=C/[C@@H](C)C(O)=O	н.»~~~у	NGGONIG-ON-CI	HO O Br R	0C([C@H](C)Br)=0.[R]
20	130124051502260417042803	12	HM~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(OCO2)C2=C1	0 O OH	OC(C1=COC(CCI)=N1)=0	H _M M	NCCNC(C)=O	۲	OC(C1=CC=C(CCl)C=C1)=0	""	NCCCN1C=CN=C1	HO O Br R	0C([C@H](C)Br)=0.[R]
24	130324101501260417022803	12	HN	C1CNCCN1	O= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ~ H ₂ O	NCCNC(C)=O	J.C.	OC(C1=CC=C(CCI)C=C1)=O	···~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	*° ¹ 07°	CICC1=CC(C(0)=0)=CC=C1
25	130424011503260517032802	12	H _I N O Br	NCC1=CC=CC(Br)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	e for the second	OC(C1=CC=C(CCl)C=C1)=O	H ₂ N OH	NCCO	HO O S	0C([C@H](C)Cl)=0.[S]
29	130424031509260317092804	11	H _. N~~0	NCCCOC	HO ^L Y ^L Y	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN TO Y	NCC1=CC=CC(C(F)(F)F)=C1	····	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
28	130424031504260817022803	11	H,M O	NCCCOC	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1	orto OH CI	OC(C1=CSC(CCI)=N1)=O	**~~\D	NCCCN1C=CN=C1	"	CICC1=CC(C(0)=0)=CC=C1
27	130124031504260417032803	11	H,N O	NCCCOC	O → → → → → → → → → → → → →	OC(C1=COC(CCI)=N1)=O	H ₂ N N YO	NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O	ни~~^rО́	NCCCN1C=CN=C1	HO O S	0C([C@H](C)Cl)=0.[S]
30	131024021501200217012808	11	H _i N (),	NUC1=CC(F)=C(F)C=C1	Hologra	CIUC1=CC(C(O)=O)=CC=C1		NUC1=CC=C(S(=O)(C)=O)C=C1	CI CH CH	UC(C1=COC(CCI)=N1)=O	H ₂ N	BICT=CC=C(CN)C=C1	O= OH	00(C1=C3C(CCI)=N1)=0
32	130124051509260317032807	10	HAN	NGC1=GC=C(OCO2)C2=C1		UU(C1=CUC(CCI)=N1)=O	in the second second	NUG1=CC=CC(C(F)(F)F)=C1	₩Î r if~o	UUUU(U)=U[C@@H](C)C(O)=O	\sim	NUGT=CC(OC)=CC	HO O S	uu[U@H](U)Cl)=O.[S]
33	130124071502260417092803	10	NH ₂	NUC1=CC=C(C)C=C1		UC(C1=COC(CCI)=N1)=O	H _M N	NGCNC(C)=0	° La Constantina de la Constan	UG(C1=CC=C(CCI)C=C1)=O	H _N N R	N[U@H](C)C1=CC=CC=C1.[R]	HO O S	uci[C@H](C)Cl)=0.[S]
34	130324031509260217102804	10	H_N 0	NCCCOC	O= OH	OC(C1=CSC(CCI)=N1)=O	HAN OF	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N S	N[C@@H](C)C1=CC=CC=C1.[S]	0H	U=C(0)C1=C(C)OC=C1
36	130324101502260217022803	10	HN	C1CNCCN1	JA CI	OC(C1=CSC(CCI)=N1)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C1	J. C	OC(C1=COC(CCI)=N1)=O	···~··	NCCCN1C=CN=C1	HO CO	CICC1=CC(C(O)=O)=CC=C1

35	130324051503260117022803	10	HIN COLO	NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCI)=N1)=O		Arrines-(A2) strilles		OC(C1=COC(CCI)=N1)=O	H,N~~\Q	Ammes-(AS) armes NCCCN1C=CN=C1	HOLOGY	ACIDS-(X2) strines CICC1=CC(C(0)=0)=CC=C1
37	130424051504260817022804	10	HN ()	NCC1=CC=C(OCO2)C2=C1		скис(с)=с.[с@@H](с)с(о)=0	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	носто	CICC1=CC(C(O)=O)=CC=C1
31	130124051502250417022804	10	HIN	NCC1=CC=C(OCO2)C2=C	O-OH	OC(C1=COC(CCI)=N1)=O	H _I N H	NCCNC(C)=O	᠂ᡁᢕ	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCC1=CC=CO1	HOLOCO	CICC1=CC(C(O)=O)=CC=C1
38	130124031502261017092803	9	H _i N~~0~	NCCCOC	O= OH	OC(C1=COC(CCI)=N1)=O	H _A N	NCC1=CC=C(CI)C=C1	[™] T↑~	CIC/C(C)=C/[C@@H](C)C(O)=O	H _I N F	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	0C([C@H](C)Cl)=0.[S]
45	130924031504260417092804	9	H ₂ N	NCCC1CCOCC1	O= ↓ OH	OC(C1=CSC(CCI)=N1)=O	H,N∼ ^H ✦°	NCCNC(C)=O	°↓ u	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
40	130224101509260117102804	9	HN	C1CNCCN1	HOLOCO	CICC1=CC(C(O)=O)=CC=C1	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H _N N S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	0=C(0)C1=C(C)OC=C1
41	130324101510260317102804	9		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	**	CIC/C(C)=C/[C@@H](C)C(0)=0	H,N S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
42	130424031509260217032803	9	H _i N 0	NCCCOC	*****	CIC/C(C)=C/[C@@H](C)C(O)=O	******	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/[C@@H](C)C(O)=O	···~~·D	NCCCN1C=CN=C1	HO O S	0C([C@H](C)Cl)=0.[S]
43	130424081503260717032803	9	HN	N1CCNCCC1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	Å.	NCC1=CC=C(N(C)C)C=C1	o=√H	OC(C1=CSC(CCI)=N1)=O	"." "D'	NCCCN1C=CN=C1	HO O S	oc([c@H](c)cl)=0.[S]
44	130924031501260917032804	9	H _I N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	HAN OF Y	NCC1=CC(F)=CC(C(F)(F)F)=C1	OF OH	OC(C1=CSC(CCI)=N1)=O	H2N	NCC1=CC=CO1	S D O	oc([c@H](c)ci)=0.[S]
39	130124091501261017032802	9	нл ^о су	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H _A N Cong	NCC1=CC=C(CI)C=C1	no for the second	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ⁻ OH	NCCO	HO_O CI S	oc([C@H](C)Cl)=0.[S]
46	130124031503260417092804	8	H ^I N 0	NCCCOC		OC(C1=COC(CCI)=N1)=O	H _I N~ ^H /°	NCCNC(C)=O	° La Corre	OC(C1=CC=C(CCI)C=C1)=O	R R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
49	130124051503280617092804	8	HAN	NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1	° L C C C C C C C C C C C C C C C C C C	OC(C1=CC=C(CCI)C=C1)=O	R R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
59	130424081509260317102804	8		N1CCNCCC1	HOLIN	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN TOX	NCC1=CC=CC(C(F)(F)F)=C1	₩ ^l tri~	CIC/C(C)=C/[C@@H](C)C(O)=O	HANK S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	0=C(O)C1=C(C)OC=C1
48	130124051501261017102804	8		NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCI)=N1)=O	HAN	NCC1=CC=C(CI)C=C1	···	CIC/C(C)=C/[C徽徽H](C)C(O)=O	the state of the s	N[C@@H](C)C1=CC=CC=C1.[S]	of the second se	0=C(O)C1=C(C)OC=C1
63	130324071601260617102804	8	NH ₂	NCC1-CC-C(C)C-C1	O=OH	OC(C1-CSC(CCI)=N1)=O	H ₂ N / OH	NCC(C)(C)O	° tu	OC(C1-CC-C(CCI)C-C1)-O	the state of the s	N[C@@H](C)C1-CC-CC-C1.[S]	of the second se	0-C(0)C1-C(C)OC-C1
55	130424031504260617032803	8	H _I M O	NCCCOC	"h	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1=CC=CC=C1	ົ້	OC(C1=CC=C(CCI)C=C1)=O	n,n~~nQv	NCCCN1C=CN=C1	HO CI S	oc([c@H)(c)ci)=0.[s]
58	130424071502260217022603	8	NH,	NCC1=CC=C(C)C=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=O)(C)=O)C=C1	OF CH	OC(C1=COC(CCl)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO LOTO	CICC1=CC(C(0)=0)=CC=C1
60	130424091504260617022803	8	"" "D	NCCCN1C=CN=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	° t (C) ~ °	OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO ^L OCTO	CICC1=CC(C(0)=0)=CC=C1
57	130424051502280417032803	8	HAN COLO	NCC1=CC=C(0CO2)C2=C1	#0 ~~~ ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	CIC/C(C)=C/[C@@H](C)C(O)=O	H _I N H _I O	NCCNC(C)=O	° L	OC(C1=CC=C(CCI)C=C1)=O	+.x~~~ny	NCCCN1C=CN=C1	HO O S	oc([C@H](C)Cl)=0.[S]
52	130224041504260717022803	8	NH ₂	NCC=C	****	CICC1=CC(C(O)=O)=CC=C1	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H.N~~N_DV	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=C1
50	130124051509260317022803	8	HAN COLO	NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCI)=N1)=O	na Ch	NCC1=CC=CC(C(F)(F)F)=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N~~N_D	NCCCN1C=CN=C1	Hologra	CICC1=CC(C(O)=O)=CC=C1
61	130424101501260617032609	8	HN	CICNCCNI	*****	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1-CC-CC-C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	0C(C1-CC-C(CCI)C-C1)-0	H ₂ N	NCC1CCOCC1	HO CI S	oc([c@H)(c)c)=o.[6]
56	130424031504260917022809	8	H,M O	NCCCOC	" ^L the	CIC/C(C)=C/[C@@H](C)C(O)=O	nn th	NCC1=CC(F)=CC(C(F)(F)F)=C1	C → C → C → C → C → C → C → C → C → C →	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1		CICC1=CC(C(0)=0)=CC=C1
47	130124031504260817032809	8	H ^I N~~O~	NCCCOC		OC(C1=COC(CCI)=N1)=O	C NH,	N[C@@H](C)C1=CC=CC=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H ₃ N	NCC1CCOCC1	HO O S	oc([c@H](c)ci)=0.[s]
54	130424031504260517032802	8	H _i N~~0~	NCCCOC	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	€ C	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	oc([C@H](C)Cl)=0.[S]
51	130224031502260817022802	8	H ₂ N~~0~	NECCOC	HO	GIGC1=GG(G(0)=O)=GG=G1		N(C@@H)(C)C1=CC=CC=C1	OF OH	00(01=050(00)=N1)=0	H ₂ N OH	NGCO	#* ¹	0001=00(0(0)=0)=00=01
66	130424071502260317032805	7	NH ₂	NCC1=CC=C(C)C=C1	HO TOTO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1	< ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=COC(CCl)=N1)=O	HAM TO	NCC1COC(C=CC=C2)=C2O1	HO C S	oc([C@H](C)Cl)=0.[S]
70	130924041501260417092804	7	H ₄ N	NCCC1CCOCC1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~ ^H / ^O	NCCNC(C)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	R R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
03	130124071502200017092804	7	NH ₂	NCC1=CC=C(C)C=C1	O= OH	OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC	°↓ CH	0C(C1=CC=C(CCI)C=C1)=0	H.N.S. R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
71	131024021503260417102804	7	H ₂ N	NCC1=CC(F)=C(F)C=C1	"" ¹ 0~"	CICC1=CC(C(O)=O)=CC=C1	н, N~^Дто	NCCNC(C)=O	° t () ° (0C(C1=CC=C(CCI)C=C1)=0	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	0=C(0)C1=C(C)OC=C1
65	130424031501261017022803	7	H ₂ N*~~~0~	NCCCOC	но	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N^	NCC1=CC=C(CI)C=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	HO ^L CT O	CICC1=CC(C(0)=0)=CC=C1
67	130424071509260417032803	7		NCC1=CC=C(C)C=C1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN OF	NCC1=CC=CC(C(F)(F)F)=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	нм~~~Ю́у	NCCCN1C=CN=C1	HO O S	0C([C@H](C)Cl)=0.[S]
68	130424091502260317032803	7	H ₂ N N	NCCCN1C=CN=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1	OF OH CI	OC(C1=COC(CCI)=N1)=O	H.M~~YOY	NCCCN1C=CN=C1	HO O S	0C([C@H](C)Cl)=0.[S]

62 62	130124031502260217032803	7	H ₁ N ⁰	NCCCOC		OC(C1=COC(CCI)=N1)=O	North	Armines-(A2) similes Ad CC1=CC=C(S(=0)(C)=0)C=C1	OH	ACIOS-(A2) stitues OC(C1=COC(CCI)=N1)=0	H,N~~N_D	Armines-(AS) strilles NCCCN1C=CN=C1		OC([C@H](C)CI)=O.[S]
69	130924031501280717042803	7	H ₂ N~	NCCC1CCOCC1	O= OH	oc(c1=cSc(cCl)=N1)=O	NH ₂ N	CC1=CC=C(N(C)C)C=C1	СН СI	0C(C1=CSC(CCI)=N1)=0	H.N~~N_DN	NCCCN1C=CN=C1	HO O R	0C([C@H](C)Br)=0.[R]
64	130324051504260817032803	7	HIN	NCC1=CC=C(OCO2)C2=C	O-CI OH	OC(C1-CSC(CCI)-N1)=0		сеени(с)с1-сс-сс-с1	СН СН	OC(C1=C8C(CCI)=N1)=O	H.N~~N_0	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[8]
84	130424031503260517092804	6	H ^I N~~0~	NCCCOC	₩ ^Î ₹`\	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H.N.S. R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	0=(0)222
85	130424051509260217092804	6		NCC1=CC=C(OCO2)C2=C1	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O	UY N	CC1=CC=CC(C(F)(F)F)=C1	~ ~	CIC/C(C)=C/[C@@H](C)C(0)=O	H.N.S. R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
75	130124071502260317092804	6	NH2	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	∧_>	cc1=cc=cs1	ото сі Сн	OC(C1=COC(CCI)=N1)=O	H.N.S. R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
81	130324061503260417092804	6	H ₂ N	NCC1=CC=CO1	CI CI CH	OC(C1=CSC(CCI)=N1)=O	√¦_∽ [№]	CCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H,N	N[C@H](C)C1=CC=CC=C1.[R]	СН	O=(0)222
77	130224041501260517102804	6	NH ₂	NCC=C	HO ^L CCCO	CICC1=CC(C(O)=O)=CC=C1		CC(C)(C)O	0	OC(C1=CC=C(CCI)C=C1)=O	H.N.S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
79	130224081503260417102804	6	HN	N1CCNCCC1	HOLING	CICC1=CC(C(O)=O)=CC=C1	~ ^H ro	CCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	Hart s	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(0)C1=C(C)OC=C1
76	130124071504260217102804	6	NH,	NCC1=CC=C(C)C=C1	OF OH	OC(C1=COC(CCI)=N1)=O	ay "	CC1=CC=C(S(=O)(C)=O)C=C1	С С С С С С С С С С С С С С С С С С С	0C(C1=COC(CCI)=N1)=0	HNY s	N[C@@H](C)C1=CC=CC=C1.[S]	OH O	O=C(0)C1=C(C)OC=C1
82	130324081509260217102804	6		N1CCNCCC1	O= OH	OC(C1=CSC(CCI)=N1)=O	UX	CC1=CC=CC(C(F)(F)F)=C1	* *~	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.Y	N[C@@H](C)C1=CC=CC=C1.[S]	OH O	O=C(O)C1=C(C)OC=C1
88	130924031502261017102804	6	H ₂ N	NCCC1CCOCC1	O= OH	OC(C1=CSC(CCI)=N1)=O		CC1=CC=C(CI)C=C1	**	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
83	130424031502260217032803	6	H _. M O	NCCCOC	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	۳ مرا	CC1=CC=C(S(=O)(C)=O)C=C1	OH CI	OC(C1=COC(CCl)=N1)=O	***~~~NOV	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
78	130224081502260717032803	6		N1CCNCCC1	но	CICC1=CC(C(O)=O)=CC=C1	,NHL N	CC1=CC=C(N(C)C)C=C1	S N OH	OC(C1=CSC(CCI)=N1)=O	"" "D	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
87	130924021501260317032803	6	H ₂ N~O	NCCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=C1	∧ ∧	CC1=CC=CS1	он он	OC(C1=COC(CCI)=N1)=O	n.x~~n_)v	NCCCN1C=CN=C1	HO O S	0C([C@H](C)Cl)=0.[S]
73	130124041501261017022803	6	NH ₂	NCC-C	O= OH	0C(C1-C0C(CCI)-N1)-0		CC1-CC-C(CI)C-C1	* *	CIC/C(C)-C/[C@@H](C)C(0)-0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NGGGN1C-GN-G1	HOLICO	CICC1-CC(C(0)-0)-CC-C1
72	130124031502261017032803	6	H _I M O	NCCCOC	O=CI OH	0C(C1=C0C(CCI)=N1)=0		cc1=cc=c(ci)c=c1	~ ~~	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M~~N_0V	NCCONTC=CN=C1	HO O S	0C([C@H](C)CI)=0.[S]
74	130124051510260317032803	6		NCC1=CC=C(OCO2)C2=C1	O-CI	0C(C1=C0C(CCI)=N1)=0	∽ _{NH₂} C	C(C)CCN	* *	CIC/C(C)=C/[C@@H](C)C(0)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=0.[S]
80	130324041502260417042803	6	MH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	~ ^H ro	CCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	~~~D	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
89	130924031503261017032803	6	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O		CC1=CC=C(CI)C=C1	**	CIC/C(C)=C/[C@@H](C)C(0)=0	n.x~~n_y	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=0.[S]
90	131024011504260617042809	6	H ₂ N	NCC1=CC(F)=C(F)C=C1	O OH	0C(C1=C0C(CCI)=N1)=0	NH ₂	CC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	HĨN	NCC1CCOCC1	HO CO R	OC([C@H](C)Br)=O.[R]
86	130424101509260217022804	6	HN	C1CNCCN1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O		CC1=CC=CC(C(F)(F)F)=C1	**	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HOLOCO	CICC1=CC(C(0)=0)=CC=C1
91	131024031504260517032802	6	H ₂ N	NCC1-CC(F)-C(F)C-C1	O= OH	0C(C1-CSC(CCI)-N1)-0		CC(C)(C)O		0C(C1-CC-C(CCI)C-C1)-0	H ₂ N	NCCO	HO O S	0C([C@H](C)CI)=0.[5]
125	130424031502260417022805	5	н,м~~о~	NCCCOC	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	- ^N o	CCNC(C)=0		0C(C1=CC=C(CCl)C=C1)=0	H,N C	NCC1COC(C=CC=C2)=C2O1	"'	CICC1=CC(C(0)=0)=CC=C1
122	130324101502260417032801	5	HN	C1CNCCN1	O= OH	OC(C1=CSC(CCI)=N1)=O	~ ^H ~°	CCNC(C)=0	0	OC(C1=CC=C(CCI)C=C1)=O	H,N Contraction	NGCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=0.[S]
113	130224101502261017092804	5	HN NH	C1CNCCN1	HOLOCO	CICC1=CC(C(O)=O)=CC=C1		CC1=CC=C(CI)C=C1	**	CIC/C(C)=C/[C@@H](C)C(O)=O	HN R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
126	130424031504260417102803	5	H ₂ N~~_0	NCCCOC	но	CIC/C(C)=C/[C@@H](C)C(O)=O	~ ^H ~ ⁰	CCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H.N.S.	N[C@@H](C)C1=CC=CC=C1.[S]	HO O S	OC([C@H](C)Cl)=O.[S]
128	130424051504261017102804	5	***	NCC1=CC=C(OCO2)C2=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O		CC1=CC=C(CI)C=C1	r	CIC/C(C)=C/[C@@H](C)C(0)=0	H.N.	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
110	130224081510260317102804	5		N1CCNCCC1	HOLOCO	CICC1=CC(C(O)=O)=CC=C1		C(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	HAN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	0=C(0)C1=C(C)0C=C1
111	130224091504200017102804	5	"" "	NCCCN1C=CN=C1	HOLOGO	CICC1=CC(C(0)=0)=CC=C1	NH ₂	CC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H.N.S	N[C@@H](C)C1=CC=CC=C1.[3]	OH OH	O=C(O)C1=C(C)OC=C1
134	131024021501261017102804	5	H ₂ N	NCC1=CC(F)=C(F)C=C1	"" ¹ 0~"	CICC1=CC(C(0)=0)=CC=C1		CC1=CC=C(CI)C=C1	14-0	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.Y.	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(0)C1=C(C)OC=C1
135	131024021502260617102804	5	H ₁ N	NCC1=CC(F)=C(F)C=C1	но	CICC1=CC(C(O)=O)=CC=C1	NH ₂	CC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	HJN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
99	130124071504260417102804	5		NCC1=CC=C(C)C=C1		0C(C1=COC(CCI)=N1)=0	√ ^l ↓o	CCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H.N.S	N[C@@H](C)C1=CC=CC=C1.[S]	0H	O=C(O)C1=C(C)OC=C1
131	130424101504260317032803	5	HN	C1CNCCN1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	∧ √ √ √	CC1=CC=CS1	OH CI	OC(C1=COC(CCI)=N1)=O	"." "D"	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]

Entry 130	Molecular ID 130424091502260817032803	Copies 5	Amines (X1)	Amines (X1)- smiles NCCCN1C=CN=C1	Acids-(X1)	Acids-(X1) smiles CIC/C(C)=C/IC@@H1(C)C(O)=O	Amines-(X2)	Amines-(X2) smiles NIC@@HI(C)C1=CC=CC=C1	Acids-(X2)	Acids-(X2) smiles OC(C1=CSC(CCI)=N1)=O	Amines-(X3)	Amines-(X3) smiles NCCCN1C=CN=C1	Acids-(X3)	Acids-(X3) smiles OC(IC@H1(C)CI)=0.IS1
100		5	H,N ~~ NON		He for the second se	01010(0)-010@@r1[0)0(0)-0	S.	10881000-00-00-01	O-CH	00(01-000(00)-11)-0	H,N~~N_)		HO S	00[08:1[0]0]-0.[0]
112	130224101501260617012803	5	HN	C1CNCCN1	но	CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1	°↓,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,	OC(C1=CC=C(CCI)C=C1)=O	***~~^IQV	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
114	130224101809260317032803	5	HN	CIENCENI	HOLOGIC	CICC1=CC(C(O)=O)=CC=C1	HAN ~ ~ ~ ~ ~ ~ ~ ~	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/[C復復H](C)C(O)=O	HM~~NDV	NCCCNIC=CN=C1	HO S	oc([C@H](C)CI)=O.[S]
108	130224031502260717012803	5	H ₂ N~~0~	NCCCOC	" ¹ 0~	CICC1=CC(C(O)=O)=CC=C1	A. C. NH	NCC1=CC=C(N(C)C)C=C1	CI CI CI	OC(C1=CSC(CCI)=N1)=O	HM~~~\[]_Y	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
109	130224031502260717032803	5	H _I N O	NCCCOC	HO ^L CCC	CICC1=CC(C(O)=O)=CC=C1	-A-CO_NHI	NCC1=CC=C(N(C)C)C=C1	CI C	OC(C1=CSC(CCI)=N1)=O	""""""""""""""""""""""""""""""""""""""	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
132	130924021509260417022803	5	H _i N	NCCC1CCOCC1	HOLOGO	CICC1=CC(C(O)=O)=CC=C1	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/[C@@H](C)C(0)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HOLOGO	CICC1=CC(C(O)=O)=CC=C1
106	130124101502260417042803	5		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H,N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)=O	~ _	OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
107	130124101503260417022803	5	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H ₂ N N	NCCNC(C)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	"" "D	NCCCN1C=CN=C1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=C1
95	130124071501260417032803	5	NH ₂	NCC1=CC=C(C)C=C1	CI CI	OC(C1=COC(CCI)=N1)=O	H,N~~ ^H ~	NCCNC(C)=O	and the second s	OC(C1=CC=C(CCI)C=C1)=O	H.N~~N_)	NCCCN1C=CN=C1	HO O S	oc([C@H](C)CI)=O.[S]
96	130124071501260617022803	5	NH ₂	NGC1=CC=C(G)C=G1		OC(C1=COC(CCl)=N1)=O	NH ₂	NCC1=CC=CC=C1	ູ	OC(C1=CC=C(CCI)C=C1)=O	HANNON	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=C1
98	130124071501261017042803	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O	H _A N	NCC1=CC=C(Cl)C=C1	· fr	CIC/C(C)=C/[C@@H](C)C(O)=O	HM~~YO	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
101	130124071509260417022803	5	L. Maria	NCC1=CC=C(C)C=C1		OC(C1=COC(CCl)=N1)=O	HAN	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~p	NCCCN1C=CN=C1	HOLOCO	CICC1=CC(C(O)=O)=CC=C1
103	130124091501260617022803	5	H.M.~~YY	NCCCN1C=CN=C1		OC(C1=COC(CCl)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	нл~~rDr	NCCCN1C=CN=C1	HO ¹ CCC	CICC1=CC(C(O)=O)=CC=C1
104	130124091501260717032803	5	******D*	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	A CALAN	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	···~	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)Cl)=O.[S]
92	130124051503261017042803	5	****	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCl)=N1)=O	HJN	NCC1=CC=C(Cl)C=C1	-	CIC/C(C)=C/[C微愛H](C)C(O)=O	HM~~101	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
93	130124061509260117012803	6	H,M ~ ()	NCC1-CC-C(OCO2)C2-C		OC(C1-COC(CCI)=N1)=O	HAN CONT	NCC1-CC-CC(C(F)(F)F)-C1	-	CIC/C(C)-C/[C@@H](C)C(O)-O	**~~~!Qr	NCCCN1C-CN-C1	O= OH	OC(C1-CSC(CCI)-N1)-O
94	130124051509260417032803	5	H.W^	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O		NGC1=CC=CC(C(F)(F)F)=C1	"lpyno	CIC/C(C)=C/[C@@H](C)C(O)=O	HM~~101	NCCCN1C=CN=C1	HO C S	oc([c@H](c)ci)=0.[S]
123	130324101503260417022803	5	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H,N~~ ^H ~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	""	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=C1
115	130324031503260417022803	5	H,N~~~O~	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H _J N	NCCNC(C)=O	\mathcal{A}	OC(C1=CC=C(CCI)C=C1)=O	~~~D	NCCCN1C=CN=C1	HOLON	CICC1=CC(C(0)=0)=CC=C1
120	130324071503261017022803	5	NH,	NCC1=CC=C(C)C=C1	ST C	OC(C1=CSC(CCI)=N1)=O	HIN	NCC1=CC=C(Cl)C=C1	·· lpsp	CIC/C(C)=C/[C@@H](C)C(O)=O	нл~~10)	NCCCN1C=CN=C1	Hologra	CICC1=CC(C(0)=0)=CC=C1
121	130324091510260317032803	5	·······	NCCCN1C=CN=C1	1 Alexandre	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	****	CIC/C(C)=C/[C@@H](C)C(O)=O	HM~~10)	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
117	130324051502261017042803	5	HAN	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	H _N N	NCC1=CC=C(Cl)C=C1	10 lest	CIC/C(C)=C/[C@@H](C)C(O)=0	HM~~10	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
118	130324051504260817012803	5	H.W^	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	Ŷ.	N[C@@H](C)C1-CC-CC-C1		OC(C1=CSC(CCI)=N1)=O	HM~~101	NCCCN1C-CN-C1		OC(C1-CSC(GCI)-N1)-O
119	130324051509260417042803	5	HM	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	" lp	CIC/C(C)=C/[C@@H](C)C(0)=0	нл~~Ю,	NCCCN1C=CN=C1	HOLO R	OC([C@H](C)Br)=O.[R]
124	130424031502260317032809	5	H _N	NCCCOC	HOLEY	CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HJN	NCC1CCOCC1	HO S	0C([C@H](C)Cl)=0.[S]
127	130424031504260617032809	5	H,N O	NCCCOC	ноцита	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H _i N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=O.[S]
102	130124081502260417022809	5		N1CCNCCC1	<u> </u>	OC(C1=COC(CCI)=N1)=O	H _N N~ ^H Y ^O	NCCNC(C)=O	\sim	OC(C1=CC=C(CCI)C=C1)=O	H _L N	NCC1CCOCC1	HO ^L CCC	CICC1=CC(C(0)=0)=CC=C1
100	130124071509260117022809	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	HAN TOX	NCC1=CC=CC(C(F)(F)F)=C1	···	CIC/C(C)=C/[C@@H](C)C(O)=O	HĮN	NCC1CCOCC1	HO LOS	CICC1=CC(C(0)=O)=CC=C1
105	130124091504260217022809	5	******	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	H _i N	NCC1CCOCC1	HO ^L OCO	CICC1=CC(C(0)=0)=CC=C1
133	130924031501200217032809	5	H,N~~	NCCC1CCOCC1		OC(C1=C3C(CCI)=N1)=O	HAN COL	NCC1=CC=C(3(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO O S	0C{[C@H](C)Cl)=0.[3]
97	130124071501260817032804	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	Ŷ	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N 0	NCC1=CC=CO1	HO_O_S	OC([C@H](C)Cl)=O.[S]
116	130324041509260317022804	5	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	HAR DY	NCC1=CC=CC(C(F)(F)F)=C1	ночто	CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N 0	NCC1=CC=CO1	HO ^L UCO	CICC1=CC(C(0)=0)=CC=C1
129	130424091502260217032802	5	1.1 ~ Y	NCCCN1C=CN=C1	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
181	130224101501260417022810	4	HN	C1CNCCN1	ноците	CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H / ^O	NCCNC(C)=O	CH CH	OC(C1=CC=C(CCI)C=C1)=O	HANN COL	NCCC1=CC=C(OC)C(OC)=C1	***	CICC1=CC(C(0)=0)=CC=C1

138	Molecular ID 130124031509260117032810	4		Amines (X1)- smiles		ACIGS-(X1) smiles Amines-(OC(C1=COC(CCI)=N1)=O	2) Amines-(X2) smiles NCC1=CC=CC(C(F)(F)F)=C1	Acids-(X2)	Acids-(X2) smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines-(X3)	Amines-(x3) smiles NCCC1=CC=C(OC)C(OC)=C1		Acids-(x3) smiles OC([C@H](C)Cl)=O.[S]
161	130124081502281017012810	4	HN	N1CCNCCC1		0C(C1=COC(CCI)=N1)=0	L ₀	HOLAN	СІСІС(С)=СІ(С@@Н](С)С(0)=0	HW~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCC1=CC=C(OC)C(OC)=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
204	130324101509260217042810	4	HN	C1CNCCN1	O= OH	0C(C1-CSC(CCI)=N1)=0	NCC1-CC-CC(C(F)(F)F)-C1	··· interior	CIC/C(C)=C(C@@HJ(C)C(O)=O	www.co.	NCCC1=CC=C(OC)C(OC)=C1	но	BtC1=CC=C(C(O)=O)C=C1
223	131024031501260417032810	4	HIN	NCC1=CC(F)=C(F)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	www.co.	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
227	131024031504260817032810	4	HIN	NCC1=CC(F)=C(F)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	N[C@@H](C)C1=CC=CC=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	HAN COL	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
207	130424041502260517032805	4	MH ₂	NCC=C	HOLING	CIC/C(C)=C/[C@@H](C)C(0)=0	OH NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ^o p ^o	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=O.[S]
206	130424031504260617032805	4	H ₂ N~~0~	NCCCOC	HOLIN	CIC/C(C)=C/[C@@H](C)C(O)=0	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1COC(C=CC=C2)=C2O1	HO CO S	OC([C@H](C)Cl)=O.[S]
211	130424051509260217032805	4	***	NCC1=CC=C(OCO2)C2=C	1 H0 4 4 4 1 0	CIC/C(C)=C/[C@@H](C)C(O)=O	NCC1=CC=CC(C(F)(F)F)=C1	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O	HyN	NCC1COC(C=CC=C2)=C2O1	HO O S	0C([C@H](C)Cl)=0.[S]
187	130224101504260817032805	4	HN	C1CNCCN1	но	CICC1=CC(C(0)=0)=CC=C1	N[C@@H](C)C1=CC=CC=C1	OH OH	OC(C1=CSC(CCI)=N1)=O	HIN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=O.[S]
188	130224101509260117032801	4	HN	CIENCENI	H	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1	-lp-	CIC/C(C)=C/[C@@H](C)C(O)=O		NGCC1=CNC2=CC=CC=C21	HO S	0C([C@H](C)CI)=0.[S]
170	130224071501260217032801	4	NH ₂	NCC1=CC=C(C)C=C1	" ¹ U"	CICC1=CC(C(O)=O)=CC=C1	NCC1=CC=C(S(=O)(C)=O)C=0		OC(C1=COC(CCI)=N1)=O		NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)Cl)=O.[S]
142	130124051501260417032801	4	***	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	NCCNC(C)=0	C C C C C C C C C C C C C C C C C C C	OC(C1=CC=C(CCl)C=C1)=O	H _A N	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)Cl)=O.[S]
221	130424101502261017022807	4	HN	C1CNCCN1	HOLINA	CIC/C(C)=C/[C@@H](C)C(O)=O	NCC1=CC=C(CI)C=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	γ	NCC1=CC(OC)=CC(OC)=C1	HOLDON	CICC1=CC(C(O)=O)=CC=C1
209	130424051501260517092804	4	***	NCC1=CC=C(OCO2)C2=C	1 HO ¹ T ¹	CIC/C(C)=C/[C@@H](C)C(O)=0	PH NCC(C)(C)O	م رکب د	OC(C1=CC=C(CCl)C=C1)=O	HIN R	N[C@H](C)C1=CC=CC=C1.[R]	СНО	CCC(0)=0
182	130224101501260717092804	4	HN	C1CNCCN1	HOLOCO	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=C(N(C)C)C=C1	O-CH	OC(C1=CSC(CCI)=N1)=O	R R	N(C@H)(C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
183	130224101602260417092802	1	HN	CIONCONI	HO^LCCCC	H,M~~	P ⁰	€ C C C C C C C C C C C C C C C C C C C	00(01-00-0(00))0-01)-0	R R	N[C@H](C)C1-CC-CC-C1.[R]	HOLOCO	GICC1-CC(C(0)-0)-CC-C1
1//	130224091504260417092804		1.1 ~ V					∼ CC	00(01=00=0(00)(0=01)=0	H_N C P	N[U@H](C)()1=CC=CU=C1.[K]	ОН	
222	131024021502260417092804	4	HIN	NCC1=CC(F)=C(F)C=C1	HO ¹ ()^0	CICC1=CC(C(O)=O)=CC=C1	T ⁿ	J. Correction	OC(C1=CC=C(CCl)C=C1)=O	HIN C R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
164	130124091503260617092804	4	""~~"C	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	NCC1=CC=CC=C1		OC(C1=CC=C(CCl)C=C1)=O	R R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
200	130324081509260117092804	4	HN	N1CCNCCC1	O=OH	OC(C1=CSC(CCI)=N1)=O	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/[C@@H](C)C(O)=O	R R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
208	130424041503260717102804	4	NH ₂	NCC=C	ноцить	CIC/C(C)=C/C@@H)(C)C(O)=O	NCC1=CC=C(N(C)C)C=C1	OH OH	OC(C1=CSC(CCl)=N1)=O	HIN S	N(C@@H)(C)C1=CC=CC=C1.(S)	OH OH	O=C(O)C1=C(C)OC=C1
216	130424091504260517102804	4	H,N ~ Y	NCCCN1C=CN=C1	HOLING	CIC/C(C)=C/(C@@H)(C)C(O)=O	OH NCC(C)(C)O	A CONTRACTOR	OC(C1=CC=C(CCI)C=C1)=O	J.	N(C@@H)(C)C1=CC=CC=C1.(S)	o H	0=C(0)C1=C(C)0C=C1
104	130224101502260517102804	4	HN	CICNCCNI	HO ¹	GICC1-CC(C(0)-0)-CC-C1	OH NCC(C)(C)(O)	SH CO	00(01-00-0(00)0-01)-0	s s	N(Cee)H(C)C1-CC-CC-C1[5]	of the off	0-0(0)01-0(0)00-01
100	100224101503200317102004		HN		10 10 m			· ↓ ↓ ↓ ↓		E.		o H	0-0(0)01-0(0)00-01
186	130224101503261017102804	4	HN		HOLICO	H_N		*	CIC/C(C)=C/(C@@H(C)C(O)=O	HIN S	N[C@@H](C)C1=CC=CC=C1[S]	of the	0=C(0)C1=C(C)0C=C1
176	130224081510260417102804	4	HN		HOLOCO		NH2	Holpino	CIC/C(C)=C/C@@H(C)C(O)=O	HIN S	N[C@@H](C)C1=CC=CC=C1[S]	o OH	0=C(0)C1=C(C)0C=C1
1/4	130224071509260417102803		NH ₂	NCC1=CC=C(C)C=C1	#0 ¹		×	-	CiCiC(C)=C/(C@@H(C)C(O)=O	HIN S	N(U@@H)(U)(1=UU=UU=U1[5]	HO C S	00((0@H)(C)(0)=0.[5]
169	130224051501260417102801	4	****	NCC1=CC=C(OCO2)C2=C	HO ^L	GICC1=CC(C(0)=0)=CC=C1	P ⁰		0C(C1=CC=C(CCI)C=C1)=0	the state of the s	N(C@@H)(C)C1=CC=CC=C11[S]	or OH	OC(C1=CSC(CCI)=N1)=O
162	130124081509260117102804	4	HN	N1CCNCCC1		0C(C1=C0C(CCI)=N1)=0	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/(C@@H)(C)C(O)=O	5 :	N[C@@H](C)C1=CC=CC=C1.[S]	of the	0=C(0)C1=C(C)0C=C1
130	130124021509200317102804	4	H ₂ N	NCC1=CC=CN=C1	0= OH	0C(C1=C0C(CCI)=N1)=0	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/(C@@H(C)C(O)=O	s s	N(C@@H)(C)C1=CC=CC=C1.[3]	o o o o o o o o o o o o o o o o o o o	0=C(0)C1=C(C)0C=C1
159	130124071509260417102804	4	NH ₂	NGC1=GC=C(C)C=C1			NCC1=CC=CC(C(F)(F)F)=C1	"	UUUUU=U[C@@H](C)C(O)=O	5	ми-шенис)C1=CC=CC=C1.[S]	OH OH	0=0(0)01=0(0)00=01
145	130124051502260517102804	4	***	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	OH NCC(C)(C)O	and the second s	0C(C1=CC=C(CCI)C=C1)=0	H _N	N[C@@H](C)C1=CC=CC=C1.[S]	0 OH	0=C(0)C1=C(C)OC=C1
202	130324101502260417102804	4	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	NCCNC(C)=0	of the second	OC(C1=CC=C(CCI)C=C1)=O	H _N	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
191	130324031501260417102803	4	HĮN O	NCCCOC	O=OH	OC(C1=CSC(CCI)=N1)=O			OC(C1=CC=C(CCI)C=C1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S]	HOLO	OC([C@H](C)Cl)=O.[S]

224	131024031503260317032806	4		NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCI)=N1)=O H	2N CS	Aritimes-(A2) similes Actus-(A2) NCC1=CC=CS1	OC(C1=COC(CCI)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)CI)=O.[S]
195	130324051501280417032806	4		NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCI)=N1)=O	M N Y	NCCNC(C)=0	0C(C1=CC=C(CCI)C=C1)=0		NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)CI)≡O [S]
219	130424101502260217022803	4	HN	CICNCCNI	10 Lps/~0	скак(с)-сладен)(с)с(о)-о	ny.	NCC1=CC=C(S(=O)(C)=O)C=C1	OC(C1=COC(CCI)=N1)=O		NCCCNIC-CN-C1	HOLOGIC	CICC1=CC(C(0)=0)=CC=C1
214	130424091501260317032803	4	нл	NCCCN1C=CN=C1	₩ [°] ₽ [₩] ~	CIC/C(C)=C/[C@@H](C)C(O)=O H;	N S		OC(C1=COC(CCI)=N1)=O		NCCCN1C=CN=C1	HO CI S	oc([c@H](c)ci)=0.[S]
215	130424091501260417032803	4	"" "	NCCCN1C=CN=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	N~~H~	NCCNC(C)=0	OC(C1=CC=C(CCI)C=C1)=O	~~~~¢	NCCCN1C=CN=C1	HO CI S	oc([c@H](c)ci)=0.[S]
217	130424091504261017022803	4	H.N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	no forto	CIC/C(C)=C/C@@H)(C)C(O)=0	"^	NCC1=CC=C(CI)C=C1	CIC/C(C)=C(C@@H)(C)C(O)=O		NCCCN1C=CN=C1	He Loro	CIGC1=CC(C(0)=O)=CC=C1
218	130424091509260217022803	4	"" "D	NCCCN1C=CN=C1	no la porto	CIC/C(C)=C/[C@@H](C)C(O)=O	mot	NCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C([C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	** ¹	CICC1=CC(C(O)=O)=CC=C1
189	130224101510260417022803	4	HN	CIENCENT	HO CON	CICC1=CC(C(0)=0)=CC=C1		HO TO	CiC/C(C)=Ci(C@@Hj(C)C(O)=O			HO LONG	0001=00(0(0)=0)=00=01
190	130224101510200417032803		HN	NCCCOC	***				00/01=00=0(0000=01=0			HO O S	
107	130224031304250617032603		H _e N O	NUCLUC	***		NH ₂		00(01=00=0(001)0=01)=0		NCCONIC-ON-CI	HO O S	
175	130224061304250317032503	4	HN	NICC1=00=0/00=04	" ¹ O~"	H	_e N S		00(01=000(00)=N1)=0 P0(01=00=0(00)=01)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO S	00/(08/h)(0/0)-0.(0)
172	130224071507260617042603	4	NH ₂	NCC1=CC=C(C)C=C1	HOLIN		NH ₂		00(01=00=0(001)0=01)=0	~~~~D	NCCCN1C=CN=C1	HO CO R	00/(0@h)(0b)=0.[h]
170	12022401504260917012802			NCCCN4C=CN=C1	****	H;			PC(C1=CSC(CC0=N1)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN4C-CN-C4	HO CO R	00(04-020/00)-0(4)
180	130224091510260317022803	4	H.M.~~YO	NCCCN1C=CN=C1	*°	CICC1=CC(C(O)=O)=CC=C1	Strength Str		CICIC/CI=C/IC@@HI/CIC/CIO=0	••~~`D	NCCCN1C=CN=C1	OF CI	CICC1=CC(C(0)=0)=CC=C1
168	130224061601260217022803	4	10,1 ~ 10,1	NCC1-CC-C(OCO2)C2-C1	#0 ¹	CICC1-CC(C(Q)-Q)-CC-C1		NCC1-CC-C(S(-0)(C)-0)C-C1	OC(C1-COC(CC)-N1)-O		NCCCN1C-CN-C1	He L	CICC1-CC(C(0)-0)-CC-C1
139	130124041502260417032803	4	HM ()	NCC=C		PU P	ny.		POCICI=CC=CrCChC=C1)=O	•~~~~b	NCCCN1C=CN=C1	He Correction	OCIIC#PHICICII=0.1SI
141	130124041510280217032803	4	MH ₂	NCC=C	O= OH	0C(C1=C0C(CC0=N1)=0	M H P		CIC/C(C)=C/C@@HI(C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO S	0C((C@H)(C)C)=0.1S1
160	130124081502280217012803	4	<i>■</i> ^{NH} 2	N1CCNCCC1		OC(C1=COC(CC)=N1)=0		NCC1=CC=C(S(=0)(C)=0)(C=C1	OC(C1=COC(CC1=N1)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1		OC(C1=CSC(CC)=N1)=O
152	130124071501260817042803	4		NCC1=CC=C(C)C=C1		0C(C1=C0C(CC)=N1)=0	\sim		0C(C1=CSC(CCh=N1)=0	~~~D	NCCCN1C=CN=C1	O= OH	OCIIC@HICIBri=0.IRI
154	130124071502280317032803	4	NH ₂	NCC1=CC=C(C)C=C1	O=CH	0C/C1=C0C/CC0=N1)=0		NCC1=CC=CS1	PC(C1=C0C(CC0=N1)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO R	0C((C@H)(C)C)=0.151
155	130124071503280317032803	4		NCC1=CC=C(C)C=C1	OH CH	H;	^s N~()		DC(C1=C0C(CCh=N1)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO S	00((C@H)(C)C)=0.151
156	130124071503260717012803	4		NCC1-CC-C(C)C-C1	O=OH	H,	^s N~V ^s		00(01=080(00)=N1)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C-CN-C1		0C(C1-CSC(CC0-N1)-0
157	130124071504260917022803	4		NCC1=CC=C(C)C=C1	O= OH		NH2	NCC1=CC(F)=CC(C(F)(F)F)=C1	HOC(C1=CSC(CCI)=N1)=O	•~~~\D	NCCCN1C=CN=C1	о- ОН	CICC1=CC(C(0)=0)=CC=C1
158	130124071504260917042803	4	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CC)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC(C)=CC(C(F)(F)F)=C1	H OC(C1=CSC(CCI)=N1)=O	~~~\C>	NCCCN1C=CN=C1	***	OC([C@H](C)Br)=0.[R]
144	130124051502260417032803	4	NH ₁	NCC1=CC=C(0C02)C2=C1		OC(C1=COC(CCI)=N1)=O	" ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~ ~		0C(C1=CC=C(CCI)C=C1)=0	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	R R	OC([C@H](C)Cl)=0.[S]
148	130124051504260317042803	4	***^\$\$	NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCI)=N1)=O	N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CS1	P OC(C1=COC(CCI)=N1)=O	~~~D	NCCCN1C=CN=C1	s s	OC([C@H](C)Br)=O.[R]
151	130124051509260217022803	4	***	NCC1=CC=C(OCO2)C2=C1	O=OH	H; OC(C1=COC(CCI)=N1)=O	2N~V\$	NCC1=CC=CC(C(F)(F)F)=C1	H CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	R R	CICC1=CC(C(0)=0)=CC=C1
194	130324041502260217032803	4	***~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC=C	о-он	OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=0)(C)=0)C=C1	H OC(C1=COC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	** ¹ 000	0C([C@H](C)Cl)=0.[S]
203	130324101504201017032803	4	NH ₂	C1CNCCN1	O=OH	0C(C1=C3C(CCI)=N1)=0	~ Qy	NCC1=CC=C(CI)C=C1	H CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~\D	NCCCN1C=CN=C1	s s	0C([C@H](C)Cl)=0.[3]
192	130324031501280717032803	4	HN	NCCCOC	O=OH	Hg OC(C1=CSC(CCI)=N1)=O	×~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(N(C)C)C=C1	OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO O	OC([C@H](C)CI)=O.[S]
193	130324031509260417032803	4	H ₂ N~0	NCCCOC	O-OH	OC(C1=CSC(CCI)=N1)=O	h Come	NCC1=CC=CC(C(F)(F)F)=C1	H CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	HD O	OC([C@H](C)CI)=O.[S]
199	130324081502260617022803	4	H,N~~O~	N1CCNCCC1		OC(C1=CSC(CCI)=N1)=O	"OY	NCC1=CC=CC=C1	0C(C1=CC=C(CCl)C=C1)=0	·······	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=C1
201	130324091504260217032803	4		NCCCN1C=CN=C1	O=	OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=C(S(=0)(C)=0)C=C1	OC(C1=COC(CCI)=N1)=O	Q	NCCCN1C=CN=C1	HO ¹ () ()	0C([C@H](C)CI)=0.[S]
			H,N Y		O= OH	10	ny.	o-Con	н			HO C S	a construction of the

Entry 226	Molecular ID 131024031503260417042803	4 Copies	Amines (X1)	Amines (X1)- smiles NCC1=CC(F)=C(F)C=C1	Acids-(X1)	Acids-(X1) smiles OC(C1=CSC(CCI)=N1)=O	Amines-(X2)	Amines-(X2) smiles NCCNC(C)=O	Acids-(X2)	Acids-(X2) smiles OC(C1=CC=C(CCI)C=C1)=O	Amines-(X3)	Amines-(X3) smiles NCCCN1C=CN=C1	Acids-(X3)	Acids-(X3) smiles OC([C@H](C)Br)=O.[R]
			r" 4		0=		H_N ~ H_PO		Store and the second se		HAN		Br R	
196	130324051508280117032803	4	***	NCC1=CC=C(OCO2)C2=C1	O=CH	OC(C1=CSC(CCI)=N1)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O	нм~~1Qv	NCCCN1CHCNHC1	HO O S	ос([с@H](с)сі)=0 [S]
205	130424031502250517012509	4	HJN O	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1-CC-CC-C1	∙ _{CH} CC⊂a	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCCICCOCCI	OF OH	OC(C1=CSC(CCI)=N1)=O
212	130424071501260617022809	4	NH ₂	NCC1=CC=C(C)C=C1	#0 [°] T ⁺ 0	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	" ¹ 0~	CICC1=CC(C(O)=O)=CC=C1
166	130224031502260717012809	4	H ₂ N~~_O~	NCCCOC	HO ^L CC ⁻⁰	CICC1=CC(C(O)=O)=CC=C1	A CANIN	NCC1=CC=C(N(C)C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H _k N	NCC1CCOCC1	O= OH	OC(C1=CSC(CCI)=N1)=O
173	130224071503260317032809	4	NH2	NCC1=CC=C(C)C=C1	HOLOCO	CICC1=CC(C(O)=O)=CC=C1	H ₂ N S	NCC1=CC=CS1	O-UH	OC(C1=COC(CCI)=N1)=O	H _i N	NCC1CCOCC1	HO S	oc([c@H](c)ci)=0.[S]
146	130124051502260817042809	4	***	NCC1=CC=C(OCO2)C2=C1	CI CI CI CI CI	OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	C= CH	OC(C1=CSC(CCI)=N1)=O	H _i N	NCC1CCOCC1	HO CO R	OC([C@H](C)Br)=O.[R]
197	130324051510260417032809	4	***	NCC1=CC=C(OCO2)C2=C1	O= OH	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	*	CIC/C(C)=C/[C@@H](C)C(O)=O	H _i N	NCC1CCOCC1	HO S	oc([C@H](C)Cl)=O.[S]
220	130424101502260817022804	4	HN	CIENCENI	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	Q _{NH}	N[C@@H](C)C1=CC=CC=C1	CH CH	0C(C1=CSC(CCI)=N1)=0	H ₂ N	NCC1=CC=C01	HOLOCO	CICC1=CC(C(0)=0)=CC=C1
100	130224031301250417032504		H _e N				H,N ~ H				H ₂ N O		HO S	
1/9	130224091509260317032804	4	*******	NCCUNTC=CN=C1	" ¹	00(01=00(0(0)=0)=00=01	~~OX	NCC1=CC=CC(C(F)(F)F)=C1	HOLAN	CIC/C(C)=C/(C@@H)(C)C(O)=0	H ₂ N	NCC1=CC=CO1	HO CO S	00(0@H)(0)0)=0.[5]
163	130124071301281017032804	4	NH,	NCCCN1C=CN=C1	O-CI	00(01=000(00)=N1)=0	H,N C	NCC1=CC=CC=C1	Holpston	00/01=00=0/001/0=01/0=0	H ₂ N	NCC1=CC=CO1	HO S	00/08/1/0/01-0/01
143	130124051502200017032804	4	""~~D			00(01=000(00)=N1)=0		NIC@@HVC\C1=CC=CC=C1		00(01=050(00)=01)=0	H ₂ N	NCC1=CC=CO1	HO S	00(08H)(00)=0.(3)
160	120124051501200017032804		HAN	NCC1-CC-C(0C02)C2-C	C C C C	00(01-000(00)-NI)-0	C NH,		CH CH	00(01-030(00)-N1)-0	H ₂ N	NCC1-CC-CO1	HO CO S	
225	131024031503260417032804	4		NGC1-CC/F)-C/F)C-C1		00(01-000(00)-N1)-0	, NH,		OH OH	00(01-030(00)-41)-0	H ₂ N 0	NCC1-CC-CO1	HO CO S	0010@HI(0)01-0.191
213	130424071509260217032802	4	H ₂ N ¹	NCC1=CC=C/CC=C1	OF OH	CICC/C)=C/C/M/MH/C)C/O)=O	H,N Y	NCC1=CC=CCC(F)(F)(F)=C1	° ↓ ↓ ↓ ↓ ↓	CIC/C/C)=C/C@/@H/C)C/O)=O	H ₂ N	NCCO	HO S	OCIIC@HICICI=O.ISI
210	130424051504280517032802	4	NH ₂		"into	CIC/C/C)=CIC/A/ALI/C)C/D)=D	********		~lp-j~		H ₂ N OH	NCCO	HO CO S	00/00/00/00/00/00
140	130124041504280517032802	4	HAN	NCC=C	-	00/01=000/001=N(1)=0	H ₂ N ⁻	NCC(C)(C)O	J.C.	00(01=00=0(00)(0=01)=0	H ₂ N OH	NCCO	HO S	00108010000-010
197	130124031504280517032802	4	MH ₂	NCCCOC		00(01=000(00)=11)=0	H ₂ N	NCC(C)(C)O	A COLO	00(01=00=0(00)(0=01)=0	H ₂ N OH	NCCO	HO S	00108010000-010
147	130124051503280817022802	4	H ₂ N~0	NCC1-CC-C/OCO20C2-C2	OF CH	00/01-000/000-11)-0	H ₂ N / OH	NIC@@U/U/C1-CC-CC-C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	00(01-00-0(00),0-01)-0	H ₂ N OH	NCCO	HO S	
149	130124051504280517032802	4	****	NCC1=CC=C(OCO2)C2=C1	CH CH	00(01=000(00)=N1)=0	Y _{NH}		o-CoH	00(01=00=0(00)(0=01)=0	H ₂ N OH	NCCO	HO LONG	
190	130324071504280517032802	4	H.N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NGG1-GG-G(G)G-G1	O-OH	00(01-000(00)-N1)-0	H ₂ N /	NGG(G)(G)O	STOC STOC	00(01-00-0(00)0-01)-0	H ₂ N OH	NGGO	HO CO S	00/(0a) 1/(0)0) - 0.[0]
408	130424091509260417022810	3	NH ₂	NCCCN1C=CN=C1	O=CH	CIC/C(C)=C/IC@@HI(C)C(O)=0	H ₂ N /	NCC1=CC=CC(C(F)(F)F)=C1	or the second se	CIC/C(C)=C/IC@@HI(C)C(0)=0	H ₂ N OH	NCCC1=CC=C(OC)C(OC)=C1	HO CO S	CICC1=CC(C(0)=0)=CC=C1
318	130224101501260617022810	3	H.H.~~Y_Y	C1CNCCN1	HUL AL	CICC1=CC(C(0)=0)=CC=C1	***~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CC1	m fro	0C(C1=CC=C(CC))C=C1)=0	HANN	NCCC1=CC=C(OC)C(OC)=C1	10	CICC1=CC(C(0)=0)=CC=C1
296	130224031509260417032810	3	HN	NECCOE	H ^e ly o	CICC1=CC(C(O)=O)=CC=C1	NH,	NCC1=CC=CC(C(F)(F)F)=C1	J.Cr.	CIC/C(C)=C/IC@@HI(C)C(0)=0	HIN	NCCC1=CC=C(OC)C(OC)=C1	"	0C/(C@H)(C)C)=0.1SI
305	130224051504260417032810	3	H ₂ N~0	NCC1=CC=C(OCO2)C2=C1	HOLO O	CICC1=CC(C(0)=0)=CC=C1	*****	NCCNC(C)=O	HO TO TO	OC(C1=CC=C(CCI)C=C1)=O	www.co	NCCC1=CC=C(OC)C(OC)=C1	HO CO S	OC([C@H](C)Cl)=O.[S]
231	130124031502260317032810	3	+*****	NCCCOC	***	OC(C1=COC(CCI)=N1)=O	H _N N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HUNNA CAR	NCCC1=CC=C(OC)C(OC)=C1	HO O S	0C([C@H](C)C)=0.[S]
325	130324031502260817022810	3	H ₂ N~O	NECCOC	OH OH	OC(C1=CSC(CCl)=N1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1	OH OH	OC(C1=CSC(CCl)=N1)=O	where the second	NCCC1=CC=C(OC)C(OC)=C1	HO S	CICC1=CC(C(0)=0)=CC=C1
329	130324031504200817022810	3	HJN	NCCCOC	O= OH	OC(C1=C3C(CCI)=N1)=O	KNH,	N[C@@H](C)C1=CC=CC=C1	O=	OC(C1=C3C(CCl)=N1)=O	HANNA COL	NCCC1=CC=C(OC)C(OC)=C1	******	CICC1=CC(C(0)=0)=CC=C1
417	130424101504260617032805	3	H,N O	C1CNCCN1	0-UN	CIC/C(C)=C/[C@@H](C)C(0)=0	KNH,	NCC1=CC=CC=C1	о	0C(C1=CC=C(CCI)C=C1)=0		NCC1COC(C=CC=C2)=C2O1		OC([C@H](C)Cl)=O.[S]
398	130424081510260417022805	3	HN	N1CCNCCC1	H0-17-4-0	CIC/C(C)=C/[C@@H](C)C(O)=0	NH ₂	CC(C)CCN	CH CO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1	× s	CICC1=CC(C(0)=0)=CC=C1
407	130424091509260317032805	3		NCCCN1C=CN=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1	H0 0	OC([C@H](C)CI)=O.[S]
292	130224031501260617022805	3	in Di	NCCCOC	HOLING	CICC1=CC(C(O)=O)=CC=C1	HAN DY	NCC1=CC=CC=C1	HO TO TO	0C(C1=CC=C(CCI)C=C1)=0	5	NCC1COC(C=CC=C2)=C2O1	s s	CICC1=CC(C(0)=0)=CC=C1
			H _I N 0		HO CO		NH ₂		et al a				"	

Entry	Molecular ID	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
311	1302240/150126101/032805	3	NH ₂	NCC1=CC=C(C)C=C1	HOLOGIC	CICC1=CC(C(0)=0)=CC=C1	H _i N	NCC1=CC=C(CI)C=C1	-	ССС(С)=С/С@@H(С)C(O)=O	HAN	NCC1COC(C=CC=C2)=C2O1	HO S	00([0@H](0)0)=0.[5]
316	130224091502260717032805	3	H,N Y Y	NCCCN1C=CN=C1	HOLIN	CICC1=CC(C(O)=O)=CC=C1	Å.	NCC1=CC=C(N(C)C)C=C1	C CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ⁻	NCC1COC(C=CC=C2)=C2O1	HO O S	ос([с@H](с)сі)=0 [S]
288	130124101504281017012805	3	HN	CICNCCNI		OC(C1=COC(CCI)=N1)=O	H,N C	NCC1=CC=C(CI)C=C1	"	СК/С(С)=С([С@@H](С)С(О)=О	HAN	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
267	130124081501260517032805	3	HN	N1CCNCCC1		OC(C1=COC(CCI)=N1)=O		NCC(C)(C)O	γ	OC(C1=CC=C(CCI)C=C1)=O	HĮN	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=O.[S]
243	130124051501260917022805	3	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(OCO2)C2=C1		OC(C1=COC(CCI)=N1)=O	•••••• <u>></u>	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H,N Y	NCC1COC(C=CC=C2)=C2O1	HO ^Î LINO	CICC1=CC(C(0)=0)=CC=C1
365	130324101504260617032805	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H _i N	NCC1COC(C=CC=C2)=C2O1	HO S	0C([C@H](C)Cl)=0.[S]
397	130424081504260417032801	3		N1CCNCCC1	HO HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~ ^H Y ^O	NCCNC(C)=O	~_^^~~	OC(C1=CC=C(CCI)C=C1)=O	B	NCCC1=CNC2=CC=CC=C21	HO S	0C([C@H](C)Cl)=0.[S]
323	130224101510260317032801	3	HN	C1CNCCN1	***	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	Bat	NCCC1=CNC2=CC=CC=C21	HO O S	0C([C@H](C)Cl)=0.[S]
233	130124031503260817032801	3	H _N N O	NCCCOC	<u></u>	OC(C1=COC(CCI)=N1)=O	Ŷ	N[C@@H](C)C1=CC=CC=C1	<u> </u>	OC(C1=CSC(CCI)=N1)=O		NCCC1=CNC2=CC=CC=C21	HO_O_S	0С([C@H](C)CI)=0.[S]
254	130124071501260617032801	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		NCCC1=CNC2=CC=CC=C21	2 O OH	ОС([C@H](C)CI)=0.[S]
349	130324071509260417032801	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	B	NCCC1=CNC2=CC=CC=C21	HOOS	0C([C@H](C)Cl)=0.[S]
302	130224051503260417032807	3	***	NCC1=CC=C(OCO2)C2=C1		CICC1=CC(C(O)=O)=CC=C1	H _I N~ ^H	NCCNC(C)=O	γ	OC(C1=CC=C(CCI)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1	HOLOS	0C([C@H](C)Cl)=0.[S]
382	130424041503260417092803	3	NH ₂	NCC=C	+0 ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~ ^H	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H _N N _R	N[C@H](C)C1=CC=CC=C1.[R]	HOLOS	0C([C@H](C)Cl)=0.[S]
372	130424031501260417092804	3	H ₂ N~0	NCCCOC	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~ ^H	NCCNC(C)=O	γ	OC(C1=CC=C(CCI)C=C1)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	~ р	CCC(0)=0
373	130424031501261017092804	3	H _L N~0	NCCCOC	#0 ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N^CC	NCC1=CC=C(Cl)C=C1	-	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]		CCC(0)=0
377	130424031503261017092803	3	HIN O	NCCCOC		СІС/С(С)-С/[С@@H](С)С(О)-О	H _N	NCC1-CC-C(CI)C-C1		CIC/C(C)-C/[C@@H](C)C(O)-O	H ₂ N _K R	N[C@H](C)C1-CC-CC-C1.[R]	HO_O_S	0C([C@H](C)Cl)=0.[8]
395	130424081503260417092804	3		N1CCNCCC1	"	СІС/С(С)=С/[С@@H](С)С(О)=О	H ₂ N~ ^H + ^O	NCCNC(C)=O	γ	OC(C1=CC=C(CCI)C=C1)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	00000
435	130924041510260117092804	3	н,м	NCCC1CCOCC1	HOTATO	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	-	CIC/C(C)=C/[C@@H](C)C(O)=O	HIN R	N[C@H](C)C1=CC=CC=C1.[R]	∕ µ⁰	O=(0)=0
403	130424091502260517092804	3	~D	NCCCN1C=CN=C1	*****	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	γ	OC(C1=CC=C(CCI)C=C1)=O	H,N K R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(0)=0
447	131024041503260417092804	3	H _I N	NCC1=CC(F)=C(F)C=C1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O	H _I N H _I O	NCCNC(C)=O	\sim	OC(C1=CC=C(CCI)C=C1)=O	H _N R	N[C@H](C)C1=CC=CC=C1.[R]		0=(0)222
390	130424051509260117092803	3		NCC1=CC=C(OCO2)C2=C1	1 HO ^L TA	CIC/C(C)=C/[C@@H](C)C(O)=O	****	NCC1=CC=CC(C(F)(F)F)=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.K. R	N[C@H](C)C1=CC=CC=C1.[R]	HO S	0C([C@H](C)Cl)=0.[S]
297	130224041504260417092804	3	NH ₂	NCC=C	***	CICC1=CC(C(O)=O)=CC=C1	H _I N H	NCCNC(C)=O	γ	OC(C1=CC=C(CCI)C=C1)=O	H,N K	N(C@H)(C)C1=CC=CC=C1.[R]	ОН ОН	CCC(0)=0
298	130224041500260217092804	3	NH ₂	NCC-C	HO ^L CCC	CICC1-CC(C(O)-O)-CC-C1	HAN THE	NCC1=CC=CC(C(F)(F)F)=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN K	N[C@H](C)C1-CC-CC-C1.[R]	ОН	CCC(0)=0
324	130224101510260317092804	3	HN	C1CNCCN1	1	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H _N A R	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	0=(0)200
308	130224061503260817092804	3	H ₂ N	NCC1=CC=CO1	^{nol} y o	CICC1=CC(C(O)=O)=CC=C1	9	N[C@@H](C)C1=CC=CC=C1	<u> </u>	OC(C1=CSC(CCI)=N1)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	→ ^O H	CCC(0)=0
310	130224071501260517092804	3		NCC1=CC=C(C)C=C1	HO TO O	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O	OH CAL	OC(C1=CC=C(CCI)C=C1)=O	H,N K R	N[C@H](C)C1=CC=CC=C1.[R]	OH	0=(0)222
423	130924021504260717092804	3	н,л	NCCC1CCOCC1	*°	CICC1=CC(C(O)=O)=CC=C1	40.00	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	O=(0)=0
425	130924021509260417092804	3	н,л	NCCC1CCOCC1	***	CICC1=CC(C(O)=O)=CC=C1	HAN TOX	NCC1=CC=CC(C(F)(F)F)=C1	H RANGE	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.K. R	N[C@H](C)C1=CC=CC=C1.[R]		0=(0)222
240	130124041504280417092804	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H Y ^O	NCCNC(C)=O	γ	OC(C1=CC=C(CCI)C=C1)=O	H _P N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	0=(0)222
230	130124031501200417092804	3	H,N O	NCCCOC		OC(C1=COC(CCI)=N1)=O	H _e N H	NCCNC(C)=O	\sim	OC(C1=CC=C(CCI)C=C1)=O	H _N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
270	130124081503260517092804	3	HN	N1CCNCCC1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	γ	OC(C1=CC=C(CCI)C=C1)=O	H _N N L n	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
258	130124071501260917092804	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	HAR OF	NCC1=CC(F)=CC(C(F)(F)F)=C1	J. Co	OC(C1=CSC(CCI)=N1)=O	H_N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
260	130124071502261017092804	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H _M N CO	NCC1=CC=C(CI)C=C1	нов	CIC/C(C)=C/[C@@H](C)C(O)=O	H_N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
228	130124011502260917092802	3	H _i N Br	NCC1=CC=CC(Br)=C1		OC(C1=COC(CCI)=N1)=O	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H_N K	N[C@H](C)C1=CC=CC=C1.[R]	HO ^L CO ^{CO}	CICC1=CC(C(0)=0)=CC=C1
					UH				OH		~			

Entry	Molecular ID	Copies Amine	s (X1) Am	nines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
272	130124091501260517092802	3		(1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)0		OC(C1=CC=C(CCI)C=C1)=O	HN K	N[C@H](C)C1=CC=CC=C1.[R]	HO ^L OCO	CICC1=CC(C(O)=O)=CC=C1
276	130124091502280717092804	з н _л л~		IIC=CN=C1		OC(C1=COC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1	C CH	OC(C1=CSC(CCI)=N1)=O	R R	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	CCC(0)=0
361	130324101502260517092804	3 HN		CN1	L'	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	مرز ⁽⁾	OC(C1=CC=C(CCI)C=C1)=O	H,N K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
347	130324071503260317092804	3	NCC1=0	CC=C(C)C=C1	£ °	OC(C1=CSC(CCI)=N1)=O	H _a N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HN 5 P	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
350	130324071509260417092804	3	NCC1=0	CC=C(C)C=C1	<u> </u>	OC(C1=CSC(CCI)=N1)=O	HAN TO Y	NCC1=CC=CC(C(F)(F)F)=C1	HO ^L Y ⁴	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N C R	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	CCC(0)=0
356	130324091502260317092804	3 H ₂ N		IC=CN=C1	× ·	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HIN K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
338	130324051504260617092804	3 H _A N~	NCC1=C	CC=C(OCO2)C2=C1	£ °	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H,N G R	N[C@H](C)C1=CC=CC=C1.[R]	∽∽ро	CCC(0)=0
342	130324051510260417092804	3 H/N	NCC1=0	CC=C(OCO2)C2=C1	L'a	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	·	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N. K	N[C@H](C)C1=CC=CC=C1.[R]	∼	O=(0)222
383	130424041504260317102804	3	NH2 NCC=C	но	CH Lyng	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1	<u> </u>	OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]	o H	O=C(O)C1=C(C)OC=C1
384	130424041504260717102804	3	NCC=C	но	lprip.	CIC/C(C)=C/[C@@H](C)C(O)=O	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
371	130424031501260117102804	3 H ₂ N		ж	ly-y-o	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~~	NCCOC		OC(C1=COC(CCI)=N1)=O	Ť.	N[C@@H](C)C1=CC=CC=C1.[S]	o H	O=C(O)C1=C(C)OC=C1
378	130424031504260917102804	3	NCCCO	ю	ly-y-	CIC/C(C)=C/[C@@H](C)C(O)=O	where the second s	NCC1=CC(F)=CC(C(F)(F)F)=C1	OH	OC(C1=CSC(CCI)=N1)=O	HAN S	N[C@@H](C)C1=CC=CC=C1.[S]	o H	O=C(O)C1=C(C)OC=C1
381	130424031510260317102802	3 H ₂ M		ж	ly-	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	OH HOLANG	CIC/C(C)=C/[C@@H](C)C(0)=0		N[C@@H](C)C1=CC=CC=C1.[S]	HO ¹ CO ¹	CICC1=CC(C(0)=0)=CC=C1
392	130424061502260317102804	3 H ₂ N	NCC1=0	CC=CO1	ly-	CIC/C(C)=C/[C@@H](C)C(O)=O	H2N	NCC1=CC=CS1	J. C	OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
399	130424091501260417102804	3 нул~		HC=CN=C1	ly-	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N~~H~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	The second secon	N[C@@H](C)C1=CC=CC=C1.[S]	o OH	O=C(O)C1=C(C)OC=C1
400	130424001501260017102803	3 H ₂ N~~~		HC-CN-C1	l _r i	CIC/C(C)-C/[C@@H](C)C(O)-O	HAN YYY	NCC1-CC(F)-CC(C(F)(F)F)-C1	Jan C	OC(C1-C8C(CCI)-N1)-O		N[C@@H](C)C1-CC-CC-C1.[8]	HO S	0C([C@H](C)Cl)=0.[8]
385	130424051501260617102804	3 H,N~		CC=C(OCO2)C2=C1	ly-y-o	CIC/C(C)=C/[C@@H](C)C(O)=O	, NH ₂	NCC1=CC=CC=C1	••• •••	OC(C1=CC=C(CCI)C=C1)=O	ž.	N[C@@H](C)C1=CC=CC=C1.[S]	o H	0=C(0)C1=C(C)OC=C1
389	130424051503281017102803	3	NCC1=0	CC=C(OCO2)C2=C1	ly-	CIC/C(C)=C/[C@@H](C)C(O)=O	H ^M	NCC1=CC=C(CI)C=C1	"	CIC/C(C)=C/[C@@H](C)C(0)=0	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	HO S	OC([C@H](C)Cl)=O.[S]
293	130224031503260817102804	3 н,м	~NCCCO	ю	در ا	CICC1=CC(C(O)=O)=CC=C1	$\hat{\mathbf{Q}}$	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH O	O=C(O)C1=C(C)OC=C1
420	130924021502260717102804	3 H ₂ N	NCCC1	CCOCC1 HO	i.	CICC1=CC(C(O)=O)=CC=C1	A Com	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	o H	O=C(O)C1=C(C)OC=C1
424	130924021504260817102804	3 H _a N	NCCC1	CCOCC1 HO	i de la comercia de l	CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
317	130224091503260317102804	3 н,м ~~		HC=CN=C1	l _o	CICC1=CC(C(O)=O)=CC=C1	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O		N(C@@H)(C)C1=CC=CC=C1.(S)	of the	O=C(O)C1=C(C)OC=C1
438	131024021501260317102804	3 H ₂ N	NCC1-C	CC(F)-C(F)C-C1	i.	CICC1=CC(C(0)=0)=CC=C1	H ₂ N S	NCC1-CC-C81		0C(C1=C0C(CCI)=N1)=0		N[C@@H](C)C1-CC-CC-C1.[6]	ot ot	0-C(0)C1-C(C)0C-C1
306	130224051509260317102804	3	NCC1=0	CC=C(OCO2)C2=C1	ion.	CICC1=CC(C(O)=O)=CC=C1	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	HAN C	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
307	130224051510260217102804	3 H.N	NCC1=0	CC=C(OCO2)C2=C1	i ogo	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	*****	CIC/C(C)=C/[C@@H](C)C(0)=0	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH OH	O=C(0)C1=C(C)OC=C1
238	130124041502260417102803	3	NH ₂ NCC=C			OC(C1=COC(CCI)=N1)=O	H _N N	NCCNC(C)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	HO S	OC([C@H](C)Cl)=O.[S]
241	130124041510260317102803	3	NH ₂ NCC=C		Le la	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	-	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.S.	N[C@@H](C)C1=CC=CC=C1.[S]	HO S	OC([C@H](C)Cl)=O.[S]
284	130124101503260717102804	3 HN		CN1		OC(C1=COC(CCI)=N1)=O	A Colonia	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H.N.S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(0)C1=C(C)OC=C1
251	130124061510260317102804	3 H ₂ N	NCC1=0	CC=CO1	L'	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	the state of the s	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
252	130124071501200117102804	3	NH2 NCC1=0	CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N~	NCCOC		OC(C1=COC(CCI)=N1)=O	H.N S	N[C@@H](C)C1=CC=CC=C1.[3]	OH OH	O=C(O)C1=C(C)OC=C1
264	130124071509260117102803	3	NCC1=0	CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	in the	NCC1=CC=CC(C(F)(F)F)=C1	HO-LT-L-a	CIC/C(C)=C/[C@@H](C)C(0)=0	HIN T	N[C@@H](C)C1=CC=CC=C1.[S]	HO_O_S	OC([C@H](C)Cl)=O.[S]
437	131024011510260317102804	3 H ₂ N	NCC1=0	CC(F)=C(F)C=C1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	Holy of	CIC/C(C)=C/[C@@H](C)C(0)=0	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
360	130324101502260217102804	3 HN		CN1	£ C	OC(C1=CSC(CCI)=N1)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	HIN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(0)C1=C(C)OC=C1
327	130324031503260517102804	3 н,м	NCCCO	xc o		OC(C1=CSC(CCI)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	HANK S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	0=C(0)C1=C(C)OC=C1

Entry 352	Molecular ID 130324081503261017102804	Copies 3	Amines (X1)	Amines (X1)- smiles N1CCNCCC1	Acids-(X1)	Acids-(X1) smiles OC(C1=CSC(CCI)=N1)=O	Amines-(X2)	Amines-(X2) smiles NCC1=CC=C(CI)C=C1	Acids-(X2)	Acids-(X2) smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines-(X3)	Amines-(X3) smiles N[C@@H](C)C1=CC=CC=C1.[S]	Acids-(X3)	Acids-(X3) smiles O=C(O)C1=C(C)OC=C1
					0= OH		H ⁱ N C		-		b s		0	
353	130324081504280417102804	3	HN	N1CCNCCC1	O= OH	OC(C1=CSC(CCl)=N1)=O	H,N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)#O	S C C C C C C C C C C C C C C C C C C C	0C(C1=CC=C(CCI)C=C1)=0	n s	N[C@@H](C)C1=CC=CC=C1 [S]	OH OH	0=C(0)C1=C(C)OC=C1
355	130324081510280417102802	3		NICCNCCCI		OC(C1=C8C(CCI)=N1)=O		CC(C)CCN	"hoj~	СК-С(С)=С-(С@@H)(С)С(0)=0	H,N	N[C@@H](C)C1=CC=CC=C1.[8]	HOLOCO	CICC1=CC(G(O)=O)=CC=C1
343	130324061509260217102804	3	H ₂ N	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O	***^Q ²	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	HN S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH OH	O=C(O)C1=C(C)OC=C1
429	130924031503260817102804	3	H ₂ N~	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	Ŷ.	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H,N S	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH	O=C(O)C1=C(C)OC=C1
430	130924031504260317102804	3	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S]	OH O	0=C(0)C1=C(C)OC=C1
433	130924031510260317102802	3	H _I N	NCCC1CCOCC1	2 m	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	···	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S]	***	CICC1=CC(C(O)=O)=CC=C1
446	131024031510260417102803	3	H ₂ N	NCC1=CC(F)=C(F)C=C1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	-	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N S	N[C@@H](C)C1=CC=CC=C1.[S]	HO S	OC([C@H](C)CI)=O.[S]
332	130324051501260417102804	3	HN TT	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	H,N H,O	NCCNC(C)=O	\sim	OC(C1=CC=C(CCl)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S]	oH oH	O=C(O)C1=C(C)OC=C1
333	130324051502260617102801	3	HAY	NGC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	ູ່	OC(C1=CC=C(CCI)C=C1)=O	HIN C	N[C@@H](C)C1=CC=CC=C1.[S]		OC(C1=CSC(CCI)=N1)=O
336	130324051503260817102804	3	****	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	9	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S]	OH OH OH	O=C(O)C1=C(C)OC=C1
414	130424101502260417012806	3		C1CNCCN1	ночто	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~H ₂ 0	NCCNC(C)=O	off	OC(C1=CC=C(CCI)C=C1)=O	NH,	NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
380	130424031509260217032806	3	H_N	NCCCOC	ноцить	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN TO Y	NCC1=CC=CC(C(F)(F)F)=C1	***	CIC/C(C)=C/[C@@H](C)C(0)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO S	OC([C@H](C)Cl)=O.[S]
387	130424051502260717012806	3	***^	NCC1=CC=C(OCO2)C2=C	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	10.m	NCC1=CC=C(N(C)C)C=C1	C CH	OC(C1=CSC(CCI)=N1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
312	130224071503260417012806	3		NCC1=CC=C(C)C=C1	ноцита	CICC1=CC(C(O)=O)=CC=C1	H,M~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC(C@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
247	130124061603260417032806	3	HM ()	NCC1-CC-C(OCO2)C2-C		OC(C1-COC(CCI)-N1)-O	H,N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)-O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1-CC-C(CCI)C-C1)-O	NH ₂	NC[C@H](C)C1-CC-CC-C1	HO O S	oc([C@H](C)CI)-O.[S]
363	130324101504260617022806	3	HN	C1CNCCN1	O= OH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	0C(C1=CC=C(CCI)C=C1)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1	-1.	CICC1=CC(C(O)=O)=CC=C1
415	130424101503260617012803	3	HN	C1CNCCN1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	\mathcal{L}	OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	O=OH	OC(C1=CSC(CCI)=N1)=O
374	130424031503260217032803	3	H _N O	NCCCOC	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	~~~v)	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
379	130424031509260117042803	3	H _I N	NCCCOC	новрема	CIC/C(C)=C/[C@@H](C)C(O)=O	HUNTON	NCC1=CC=CC(C(F)(F)F)=C1	****	CIC/C(C)=Cr[C@@H](C)C(0)=0	H.N~~N_DN	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
368	130424021501260617032803	3	H ₂ N	NCC1=CC=CN=C1	10 ×	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	$\sim 0^{-1}$	OC(C1=CC=C(CCI)C=C1)=O	H.N~~N_0	NCCCN1C=CN=C1	HO S	0C([C@H](C)Cl)=0.[S]
370	130424021504260717032803	3	H ₂ N	NCC1=CC=CN=C1	ноцита	CIC/C(C)=C/[C@@H](C)C(O)=O	A CANH	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HU U S	0C([C@H)(C)Cl)=0.[S]
303	130424071501260517012803	3	NH ₂	NCC1-CC-C(C)C-C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	···~··Q·	NCCCN1C-CN-C1		OC(C1=CSC(CCI)=N1)=O
434	130924041503260317032803	3	H _i N	NCCC1CCOCC1	HU I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₅ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	***~`D	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
401	130424091502260217032803	3	1.N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	ночто	CIC/C(C)=C/[C@@H](C)C(O)=O	the second se	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	···~···	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
402	130424091502260317022803	3	"" "	NCCCN1C=CN=C1	ночто	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=C1
448	131024041504260817032803	3	H ₂ N	NCC1=CC(F)=C(F)C=C1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	1.1 ~ 1 Or	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
386	130424051502260617022803	3	HM ()	NCC1=CC=C(OCO2)C2=C		CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	~^	OC(C1=CC=C(CCI)C=C1)=O	**~~D	NCCCN1C=CN=C1	HO ¹ CCC	CICC1=CC(C(O)=O)=CC=C1
388	130424051503260217032803	3	HM ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(OCO2)C2=C		CIC/C(C)=C/[C@@H](C)C(O)=O	HAN COLOR	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	~~~^^	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
299	130224041509200417032803	э	NH ₂	NCC=C	HOLOCO	CICC1=CC(C(O)=O)=CC=C1	HAN	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=Cr[C@@H](C)C(O)=O	H.N~~N_ON	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[3]
320	130224101502260717032803	3	HN	C1CNCCN1	10 ¹ 0 ⁰	CICC1=CC(C(O)=O)=CC=C1	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H.N~~N_OV	NCCCN1C=CN=C1	HOS	OC([C@H](C)Cl)=O.[S]
294	130224031504260817032803	3	H ₂ N-~~0-	NCCCOC	HOLICO	CICC1=CC(C(O)=O)=CC=C1	P.	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	···~~··O·	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
295	130224031504261017012803	3	H ₂ N~0	NCCCOC	HOLON	CICC1=CC(C(O)=O)=CC=C1	H _A M C	NCC1=CC=C(CI)C=C1	no la grafico	CIC/C(C)=C/[C@@H](C)C(O)=O	w~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
309	130224071501260217012803	3	NH ₂	NCC1=CC=C(C)C=C1	#0 ¹	CICC1=CC(C(O)=O)=CC=C1	MAN COLOR	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	H.M.~~ 104	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O

Entry 280	Molecular ID 130224011503260717032803	Copies	Amines (X1)	Amines (X1)- smiles	Acids-(X1)	Acids-(X1) smiles	Amines-(X2)	Amines-(X2) smiles	Acids-(X2)	Acids-(X2) smiles	Amines-(X3)	Amines-(X3) smiles	Acids-(X3)	Acids-(X3) smiles
200		5	H ₂ N Br	1001-00-00(0)-01	HO ^L OO	0.001-00(0(0)-0)-00-01	A NH	1001-00-0(1(0)0)0-01	Q CH CH	00(01-000(00)-41)-0	H,N~~NQV	1000110-01-01	HO S	00[08:1[0]0]~0.[0]
422	130924021503280417032803	3	н,н~О	NCCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=C1	H _M N	NCCNC(C)=O	ୢୄ୷ୣୖ୰	OC(C1=CC=C(CCI)C=C1)=O	нл~~Ю	NCCCN1C=CN=C1	HO O S	0C([C@H](C)CI)=0.[S]
313	130224091501260417032803	3	8,0~~YCN	NCCCN1C=CN=C1	HO ¹ O ¹	CICC1=CC(C(O)=O)=CC=C1	H _L N N	NCCNC(C)=O	s and the second	OC(C1=CC=C(CCI)C=C1)=0	H,N~~YY	NGCCN1C=CN=C1	HO S	oc([C@H](C)CI)=0.[S]
314	130224091501260517032803	3	H.N~~YY	NCCCN1C=CN=C1	" ¹ 0~	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H.N~~NN	NCCCN1C=CN=C1	HO S	0C([C@H](C)Cl)=0.[S]
439	131024021503260417032803	3	H _i N Y	NCC1=CC(F)=C(F)C=C1	HO ^L CC ⁰	CICC1=CC(C(O)=O)=CC=C1	HM	NCCNC(C)=O	, () ,	OC(C1=CC=C(CCl)C=C1)=O	····~~b	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
300	130224051501260517022803	3	***	NCC1=CC=C(OCO2)C2=C1	но	CICC1=CC(C(O)=O)=CC=C1	H ₂ N H	NCC(C)(C)O	ᢩ	OC(C1=CC=C(CCI)C=C1)=O	HM~~100	NCCCN1C=CN=C1	HOLONO	CICC1=CC(C(0)=O)=CC=C1
301	130224051501260917042803	3	HN	NCC1=CC=C(OCO2)C2=C1	HO ^L	CICC1=CC(C(O)=O)=CC=C1	HAN YOY	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	44~~YO4	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
237	130124041501261017042803	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	HIN	NCC1=CC=C(CI)C=C1	HO ^L T ^S	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~D	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
283	130124101503260717032803	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1	CH CI	OC(C1=CSC(CCI)=N1)=O	H.M~~N_0	NCCCN1C=CN=C1	HO CI S	oc([C@H](C)Cl)=0.[S]
285	130124101503260817032803	3		C1CNCCN1		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H.N.~~1(3)	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
286	130124101503260817042803	3	HN	C1CNCCN1	CI CI	OC(C1=COC(CCI)=N1)=O	C K	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
287	130124101504260617032803	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1	e for the second	OC(C1=CC=C(CCI)C=C1)=O	~~~	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
232	130124031502260717032803	3	H ₂ N~~_O~	NCCCOC		OC(C1=COC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
234	130124031503260917032803	3	H ₂ N~~0~	NCCCOC	OF CI	OC(C1=COC(CCI)=N1)=O	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1	S S OH	OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)CI)=O.[S]
265	130124081501260217022803	3		N1CCNCCC1	O-CI OH	OC(C1=COC(CCI)=N1)=O	March &	NCC1=CC=C(S(=O)(C)=O)C=C1	Or CI Or CI	OC(C1=COC(CCI)=N1)=O	"" "D	NCCCN1C=CN=C1	Ho ¹ CC ⁻⁰	CICC1=CC(C(O)=O)=CC=C1
271	130124081506260317042803	3	HN	N1CCNCCC1	O=OH	OC(C1-COC(CCI)-N1)-O	HAN CAL	NCC1-CC-CC(C(F)(F)F)-C1	······································	CIC/C(C)-C/[C@@H](C)C(O)-O	~~~D	NCCCN1C-CN-C1	HO O R	OC([C@H](C)Br)=O.[R]
229	130124021502260317032803	3	H ₂ N	NCC1=CC=CN=C1	O= OH	OC(C1=COC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	o=↓ OH	OC(C1=COC(CCI)=N1)=O	~~~D	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
253	130124071501260417022803	3	NH,	NCC1=CC=C(C)C=C1	O=OH	OC(C1=COC(CCI)=N1)=O	H,N~~~ ^N ~	NCCNC(C)=O	\mathcal{L}	OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1
256	130124071501260817032803	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	~~~D	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
273	130124091501260617042803	3	~~	NCCCN1C=CN=C1	O=OH	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1	~~	OC(C1=CC=C(CCI)C=C1)=O	~~D	NCCCN1C=CN=C1	HO O R	0C([C@H](C)Br)=0.[R]
275	130124091502260417042803	3	H.M.~~ (C)N	NCCCN1C=CN=C1	O OH	OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H	NCCNC(C)=O	\sim	OC(C1=CC=C(CCI)C=C1)=O	~~~D	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
278	130124091503260517032803	3	H.M.~~\C_M	NCCCN1C=CN=C1	O-CI O-OH	OC(C1=COC(CCI)=N1)=O	H ₂ N / OH	NCC(C)(C)O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	нл~~Ю	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)CI)=O.[S]
279	130124001504260517022803	3	***~~D	NGCCN1C-CN-C1	O=OH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1-CC-C(CCI)C-C1)=O	нм~~~Ю́	NCCCN1C-CN-C1	новит	CICC1-CC(C(O)-O)-CC-C1
280	130124091504260917042803	3	1.1 ~ D	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	HAN OF	NCC1=CC(F)=CC(C(F)(F)F)=C1	CI CI CH	OC(C1=CSC(CCI)=N1)=O	1.N~~10.	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
281	130124091509260217032803	3	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	HAR DY	NCC1=CC=CC(C(F)(F)F)=C1	Holy of	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	HO S	0C([C@H](C)Cl)=0.[S]
436	131024011504260717042603	3	H ₂ N	NCC1=CC(F)=C(F)C=C1	O=CH	OC(C1=COC(CCI)=N1)=O	-L	NCC1=CC=C(N(C)C)C=C1	Q= CH CH	OC(C1=CSC(CCI)=N1)=O	""""""""""""""""""""""""""""""""""""""	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
244	130124051502260317022803	3	***~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(OCO2)C2=C1	O=OH	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	1.x~~1Q1	NCCCN1C=CN=C1	He Land	CICC1=CC(C(O)=O)=CC=C1
362	130324101503260617022803	3	HN	C1CNCCN1	ST ⊂I	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H.M.~~N_OV	NCCCN1C=CN=C1	HO ^Î () ⁽	CICC1=CC(C(O)=O)=CC=C1
366	130324101509260417042803	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	HAN TO Y	NCC1=CC=CC(C(F)(F)F)=C1	10 lest	CIC/C(C)=C/[C@@H](C)C(0)=0	HM~~101	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
354	130324081509200417032803	э		N1CONCCC1		OC(C1=C3C(CCI)=N1)=O	HAN YOY	NCC1=CC=CC(C(F)(F)F)=C1	-	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO S	0C{[C@H](C)Cl)=0.[3]
345	130324071501260817012803	3	NH ₁	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	~~~~~	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
348	130324071503260817042803	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	P	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	···~···D·	NCCCN1C=CN=C1	HO CON	OC([C@H](C)Br)=O.[R]
428	130924031501260817042803	3	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O		N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HM~~~1()/	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
432	130924031504260817022803	3	H ₂ N~	NCCC1CCOCC1	O=OH	OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H.M~~N_OV	NCCCN1C=CN=C1	HO ^L CO ^{CO}	CICC1=CC(C(O)=O)=CC=C1

359	130324091503260817022803 3	H,H~~Y	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=0			NCCCNIC=CN=C1	CICC1=CC(C(0)=0)=CC=C1
442	131024031503260817012803 3	H ₂ N	NCC1=CC(F)=C(F)C=C1	J. J. C	OC(C1=CSC(CCI)=N1)=O		0C(C1=CSC(CCI)=N1)=0	NCCCN1C#CN#C1	CI 0C(C1=CSC(CCI)=N1)=0
444	131024031809260217012803 3	H ₂ N	NGC1=CC(F)=C(F)C=C1		ос(c1=c3c(cci)=N1)=0 H.X	۲ NGC1-CC-CC(C(P)(P)P)=C1	0-(0)2(2)2-2(2)(2)2(2)2(2)2(2)2(2)2(2)2(2)2(CI 0C(C1=CSC(CCI)=N1)=0
335	130324051503260817032803 3	HANTE	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	N(C@@H)(C)C1=CC=CC=C1	0C(C1=CSC(CCI)=N1)=0	NCCCN1C=CN=C1	0C([C@H](C)Cl)=0.[S]
340	130324051509260217012803 3	HANNEL	NCC1=CC=C(OCO2)C2=C		0C(C1=CSC(CCI)=N1)=0	VCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/(C@@H)(C)C(O)=O	NCCCN1C=CN=C1	CI 0C(C1=CSC(CCI)=N1)=0
416	130424101504260617022808 3	HN	C1CNCCN1	HOLIN	CIC/C(C)=C/[C@@H](C)C(0)=0	IH2 NCC1=CC=CC=C1	0C(C1=CC=C(CCI)C=C1)=0	BrC1=CC=C(CN)C=C1	CICC1=CC(C(0)=0)=CC=C1
396	130424081503260917032808 3		N1CCNCCC1	H0 4 4 4 0	CIC/C(C)=C/[C@@H](C)C(O)=O	VCC1=CC(F)=CC(C(F)(F)F)=C1	CC(C1=CSC(CCI)=N1)=O	BrC1=CC=C(CN)C=C1	0C([C@H](C)CI)=O.[S]
259	130124071502261017022808 3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		CIC/C(C)=C/(C@@H)(C)C(O)=O	BrC1=CC=C(CN)C=C1	CICC1=CC(C(O)=O)=CC=C1
246	130124051503260417012808 3	HAN TOT	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	NCCNC(C)=O	0C(C1=CC=C(CCI)C=C1)=0	BrC1=CC=C(CN)C=C1	CI 0C(C1=CSC(CCI)=N1)=0
358	130324091503260717012808 3	H.M.	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O		0C(CT=CSC(CCI)=N1)=0	BrC1=CC=C(CN)C=C1	CI 0C(C1=CSC(CCI)=N1)=0
412	130424101501261017032809 3	HN	C1CNCCN1	HOLPSTO	CIC/C(C)=C/[C@@H](C)C(O)=O	NCC1=CC=C(CI)C=C1	CIC/C(C)=C/(C@@HJ(C)C(O)=O	NCC1CCOCC1	S
413	130424101502260217042809 3	HN	C1CNCCN1	ночто	CIC/C(C)=C/[C@@H](C)C(0)=0	NCC1=CC=C(S(=0)(C)=0)C=C1	0C(C1=C0C(CCI)=N1)=0	NCC1CCOCC1	OC([C@H](C)Br)=O.[R]
369	130424021502260817022809 3	H ₂ N	NCC1=CC=CN=C1	HOLINA		N(C@@H)(C)C1=CC=CC=C1	OC(C1=CSC(CCI)=N1)=O	NCC1CCOCC1	CICC1=CC(C(O)=O)=CC=C1
394	130424071501260517032809 3		NCC1=CC=C(C)C=C1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O	DH NCC(C)(C)O	0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	NCC1CCOCC1	OC([C@H](C)Cl)=O.[S]
391	130424051509260317022809 3	HAN	NCC1=CC=C(OCO2)C2=C		CIC/C(C)=C/[C@@H](C)C(O)=O	VCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/(C@@HI(C)C(O)=O	NCC1CCOCC1	CICC1=CC(C(0)=0)=CC=C1
321	130224101503260217032800 3	HN	C1CNCCN1	HOLOCO	CICC1-CC(C(0)-0)-CC-C1	NCC1-CC-C(S(-O)(C)-O)C-C1	00(C1-C0C(CCI)-N1)-0	NCC1CCOCC1	0C([C@H](C)CI)-0.[8]
322	130224101503260717042809 3	HN	C1CNCCN1	1	CICC1=CC(C(0)=0)=CC=C1		00C(C1=CSC(CCI)=N1)=0	HO H	OC([C@H](C)Br)=O.[R]
291	130224031501260417022809 3	H,N~~0	NCCCOC	HO ¹ U ⁻⁰	CICC1=CC(C(O)=O)=CC=C1	NCCNC(C)=0	0C(C1=CC=C(CCI)C=C1)=0	NCC1CCOCC1	CICC1=CC(C(O)=O)=CC=C1
290	130224011504260817032809 3	HN O	NCC1=CC=CC(Br)=C1	HOLOCO	CICC1=CC(C(0)=0)=CC=C1	N[C@@H](C)C1=CC=CC=C1) OC(C1=CSC(CCI)=N1)=O	NCC1CCOCC1	OC([C@H](C)Cl)=O.[S]
315	130224091502260217012809 3	H,N~~N_	NCCCN1C=CN=C1	HOLOCO	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=C(S(=0)(C)=0)C=C1	0C(C1=COC(CCI)=N1)=0	NCC1CCOCC1	CI OC(C1=CSC(CCI)=N1)=O
304	130224051504260317022809 3	HANTER	NCC1=CC=C(OCO2)C2=C		CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CS1	0C(C1=C0C(CCI)=N1)=0	NCC1CCOCC1	CICC1=CC(C(O)=O)=CC=C1
236	130124041501261017022809 3	NH	NCC=C	O= OH	OC(C1=COC(CCI)=N1)=O		CIC/C(C)=C/(C@@HI(C)C(O)=O	NCC1CCOCC1	CICC1=CC(C(O)=O)=CC=C1
235	130124031509260217012809 3	H _J N~0	NGCCOC	o= ↓ ∩ ⊂	0C(C1-COC(CCI)-N1)-0	X ^r NCC1-CC-CC(C(F)(F)F)-C1	CIC/C(C)-C(C@@11(C)C(O)-O		CI 0C(C1-CSC(CCI)-N1)-0
268	130124081502261017012809 3	HN	N1CCNCCC1		OC(C1=COC(CCI)=N1)=O		CICIC(C)=C(C@@H)(C)C(O)=O		CI 0C(C1=CSC(CCI)=N1)=0
269	130124081503260517022809 3	HN	N1CCNCCC1		0C(C1=COC(CCI)=N1)=0	DH NCC(C)(C)O	0C(C1=CC=C(CCI)C=C1)=0	NCC1CCOCC1	CICC1=CC(C(O)=O)=CC=C1
255	130124071501260717012809 3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		GC(C1=CSC(CCI)=N1)=0	NCC1CCOCC1	CI OC(C1=CSC(CCI)=N1)=O
257	130124071501260817032809 3	L) NO	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=0		I OC(C1=CSC(CCI)=N1)=O	NCC1CCOCC1	5 S
274	130124091502260317022809 3	HIN	NCCCN1C=CN=C1	O OH	OC(C1=COC(CCI)=N1)=0	S NCC1=CC=CS1	0C(C1=C0C(CCI)=N1)=0	NCC1CCOCC1	CICC1=CC(C(0)=0)=CC=C1
277	130124091502260917022809 3	ни	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=0	V NCC1=CC(F)=CC(C(F)(F)F)=C1	0C(C1=CSC(CCi)=N1)=0	NCC1CCOCC1	CICC1=CC(C(0)=0)=CC=C1
248	130124051503201017012809 3	HANTON	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	C NCC1=CC=C(CI)C=C1		NCC1CCOCC1	CI 0C(C1=C3C(CCI)=N1)=0
249	130124051504280817032809 3	HAN	NCC1=CC=C(0C02)C2=C		UC(C1=COC(CCI)=N1)=0		H ₁ N		S
250	130124051504260917012809 3	HANTER	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	X ^f NCC1=CC(F)=CC(C(F)(F)F)=C1) OC(C1=CSC(CCI)=N1)=O		CI OC(C1=CSC(CCI)=N1)=O
331	130324041503260617022809 3	NH	NCC=C	O= OH	OC(C1=CSC(CCI)=N1)=O	IH2 NCC1=CC=CC=C1	0 OC(C1=CC=C(CCI)C=C1)=0	NCC1CCOCC1	CICC1=CC(C(O)=O)=CC=C1
334	130324051503260717032809 3	HANTE	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	NH ₂ NCC1=CC=C(N(C)C)C=C1) OC(C1=CSC(CCI)=N1)=O	NCC1CCOCC1	0C([C@H](C)Cl)=0.[S]

411	Molecular ID 130424101501260817032804	3	HN NH	Amines (X1)- smiles C1CNCCN1	HOLIGS-(X1)	Acids=[X1] smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines-(X2)	Amines-(X2) smiles N[C@@H](C)C1=CC=CC=C1		Acids-(X2) smiles OC(C1=CSC(CCI)=N1)=O		Amines-(X3) smiles NCC1=CC=CO1	HO S	Acids-(X3) smiles OC([C@H](C)CI)=O.[S]
405	130424091504260417032804	3	H,M YYY	NCCCN1C=CN=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N N Y O	NCCNC(C)#O	€ CH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1	HO O S	0C([C@H](C)CI)=0.[S]
421	130924021502261017042804	3	H ₂ N	NCCC1CCOCC1	10	CICC1=CC(C(O)=O)=CC=C1	H _i N	NGC1=GC=G(GI)G=C1	-	CIC/C(C)=C(C@@H)(C)C(O)=O	H ₂ N	NGC1-CC-CO1	HO O Br R	oc([c@H](c)Br)=0.[R]
239	130124041504260417032804	3	/ NH2	NCC=C		OC(C1=COC(CCI)=N1)=O	н <u>и</u> ~ ^Д ~°	NCCNC(C)=O		OC(C1=CC=C(CCl)C=C1)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)CI)=O.[S]
263	130124071504260617022804	3		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	C NH,	NCC1=CC=CC=C1	and the second s	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N 0	NCC1=CC=CO1	HO ^L OTO	CICC1=CC(C(O)=O)=CC=C1
282	130124091509260317022804	3	H.M.~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=0	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	·	CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N	NCC1=CC=CO1	но	CICC1=CC(C(0)=0)=CC=C1
245	130124051502260417012804	3	****	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	H_N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
367	130324101510260317042804	3	HN	C1CNCCN1	C= CH	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	-	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO O R	OC([C@H](C)Br)=O.[R]
351	130324071510260317032804	3		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	Hora and a second	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO S	oc([C@H](C)Cl)=0.[S]
427	130924031501260717022804	3	H,N~	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1	CH CI	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1		CICC1=CC(C(O)=O)=CC=C1
443	131024031504260917022804	3	H ₂ N Y	NCC1=CC(F)=C(F)C=C1	J. Co	OC(C1=CSC(CCI)=N1)=O	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	" ¹ U"	CICC1=CC(C(0)=0)=CC=C1
339	130324051509260117032804	3	***	NCC1=CC=C(OCO2)C2=C		OC(C1=CSC(CCI)=N1)=O	HAN THE	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N	NCC1=CC=CO1	HO_O S	0C([C@H](C)Cl)=0.[S]
418	130424101504260817032802	3		C1CNCCN1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=0	Ŷ	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO_O S	0C([C@H](C)Cl)=0.[S]
375	130424031503260617022802	3	H ₂ N~~0~	NCCCOC	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	***	CICC1=CC(C(0)=0)=CC=C1
376	130424031503260717032802	3	H_N~~O	NCCCOC	ночто	CIC/C(C)=C/[C@@H](C)C(O)=O	A CAN	NCC1=CC=C(N(C)C)C=C1	J.	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
101	130424001502260817032802	3	H.M.~~YY	NCCCN1C-CN-C1	натра	CIC/C(C)-C/[C@@H](C)C(O)-O	Ŷ	N[C@@H](C)C1-CC-CC-C1		OC(C1-CSC(CCI)-N1)-O	H ₂ N OH	NCCO	HO S	oc([C@H](C)CI)=O.[8]
406	130424091504260517032802	3		NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N /	NCC(C)(C)O		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO_O s	0C([C@H](C)CI)=0.[S]
409	130424091510260317032802	3	n.n~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N ^{OH}	NCCO	HO_O_S	OC([C@H](C)Cl)=O.[S]
410	130424091510260417032802	3	···~··D	NCCCN1C=CN=C1	HOLPAN	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	10 min	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO_O_S	OC([C@H](C)Cl)=O.[S]
319	130224101501260617032802	3	HN	C1CNCCN1	HO	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1	~~	OC(C1=CC=C(CCl)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
419	130924021502260717032802	3	H,N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCC1CCOCC1	H0 ¹ 1270	CICC1=CC(C(O)=O)=CC=C1	A CALINA	NCC1=CC=C(N(C)C)C=C1	<u>J</u>	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
303	130224051503260817032802	3	HAY TO	NCC1=CC=C(OCO2)C2=C	1 HOLOTO	CICC1=CC(C(O)=O)=CC=C1	$\hat{\mathbf{Q}}$	N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HU O S	OC([C@H](C)Cl)=O.[S]
266	130124081501260217032802	3	HN	N1CCNCCC1		OC(C1=COC(CCI)=N1)=O	**************************************	NCC1-CC-C(S(-O)(C)-O)C-C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	oc([c@H](C)CI)=0.[6]
261	130124071503260617032802	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1	e con	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
262	130124071504260517032802	3	NH ₁	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N H	NCC(C)(C)O	$\mathcal{L}^{(r)}$	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO_O_S	OC([C@H](C)Cl)=O.[S]
242	130124051501260317032802	3	***^	NCC1=CC=C(OCO2)C2=C		OC(C1=COC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
330	130324041502260217032802	3	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=O)(C)=O)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO_O s	OC([C@H](C)Cl)=O.[S]
364	130324101504260617032802	3	HN	C1CNCCN1	J. J. C	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	CH CH	OC(C1=CC=C(CCl)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
326	130324031502260817032802	3	нулто	NCCCOC		OC(C1=CSC(CCl)=N1)=O	$\hat{\mathbf{Q}}$	N[C@@H](C)C1=CC=CC=C1	J. Co	OC(C1=CSC(CCl)=N1)=O	H ₂ N OH	NCCO	HO S	0C([C@H](C)Cl)=0.[S]
328	130324031504200517032802	3	H,N~~0~	NCCCOC	OH	OC(C1=C3C(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	OH	OC(C1=CC=C(CCl)C=C1)=O	H ₂ N OH	NCCO	HO_O_S	OC([C@H](C)CI)=O.[3]
344	130324071501260417032802	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N H ₂ O	NCCNC(C)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HOS	OC([C@H](C)Cl)=O.[S]
346	130324071502260317032802	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO_O_S	OC([C@H](C)CI)=O.[S]
426	130924031501260717022802	3	H _i N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	A NH	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO CON	CICC1=CC(C(O)=O)=CC=C1
431	130924031504260517032802	3	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	он от с	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO_O s	OC([C@H](C)Cl)=O.[S]
357	130324091503260417032802 3		NCCCN1C=CN=C1		ACIDS-(A I) STITLES OC(C1=CSC(CCI)=N1)=O	H_N N	Armines-(A2) similes		ACIDS-(AC) stitles OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	Arrines-(AS) smiles		OC([C@H](C)CI)=O.[S]	
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440	131024031501280617032802 3	H ₂ N Y	NCC1=CC(F)=C(F)C=C1	K CI	OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	€ Currore	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	oc([c@H](c)ci)≡o [S]	
441	131024031503260717032802 3	H ₂ N	NCC1=CC(F)=C(F)C=C1	СП ОН	OC(C1=CSC(CCI)=N1)=O	A COLINI	NGC1=CC=G(N(C)C)C=C1	O= UH	OC(C1=CSC(CCl)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]	
445	131024031509260317032802 3	HaN	NCC1=CC(F)=C(F)C=C1	K CI	OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CC(C(F)(F)F)=C1	₩ [°] T [†]	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N-~OH	NCCO	HO O S	0C([C@H](C)Cl)=0.[S]	
337	130324051504260517032802 3	***	NCC1=CC=C(OCO2)C2=C1		OC(C1=CSC(CCI)=N1)=O		NCC(C)(C)O	°↓ U	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]	
341	130324051509260217032802 3	HAN TOTO	NCC1=CC=C(OCO2)C2=C1	K CI	OC(C1=CSC(CCI)=N1)=O	HIN CON	NCC1=CC=CC(C(F)(F)F)=C1	···	CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]	
904	130424031502260217032810 2	H ₂ N 0	NCCCOC	i _r	CIC/C(C)=C/[C@@H](C)C(O)=O	"^Qy	NCC1=CC=C(S(=O)(C)=O)C=C1	C → CI C → CI OH	OC(C1=COC(CCI)=N1)=O	www.co	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]	
950	130424071502260517022810 2	NH ₂	NCC1=CC=C(C)C=C1	lest of	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	° La Carto de la C	OC(C1=CC=C(CCI)C=C1)=O	www.co.d	NCCC1=CC=C(OC)C(OC)=C1	HO ^Î (J ⁻)	CICC1=CC(C(O)=O)=CC=C1	
960	130424071504260817022810 2	NH ₂	NCC1=CC=C(C)C=C1	l _{yr} iya	CIC/C(C)=C/[C@@H](C)C(O)=O	Real Action of the second seco	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HUN COL	NCCC1=CC=C(OC)C(OC)=C1	ноборого	CICC1=CC(C(O)=O)=CC=C1	
984	130424091502260417032810 2		NCCCN1C=CN=C1	lysy-	CIC/C(C)=C/[C微愛H](C)C(O)=O	н,м	NCCNC(C)=O	ູ	OC(C1=CC=C(CCI)C=C1)=O	www.co.do	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]	
985	130424091502260517032810 2	***	NCCCN1C=CN=C1	l _{ri}	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	\mathcal{L}	OC(C1=CC=C(CCI)C=C1)=O	HAR COL	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)Cl)=O.[S]	
662	130224041510260417032810 2	^{NH₂}	NCC=C	Loro	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	HAR COL	NCCC1=CC=C(OC)C(OC)=C1	HO O S	0C([C@H](C)Cl)=0.[S]	
744	130224101502260917032810 2	HN	C1CNCCN1	Loro	CICC1=CC(C(O)=O)=CC=C1	nn fr	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	www.col	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]	
638	130224031501261017022810 2	H ₂ M~0	NCCCOC HO	i.	CICC1=CC(C(O)=O)=CC=C1	H,M C	NCC1=CC=C(Cl)C=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	www.col	NCCC1=CC=C(OC)C(OC)=C1	"	CICC1=CC(C(O)=O)=CC=C1	
643	130224031504260417022810 2	H ₂ N~0	NCCCOC HO	Loro	CICC1=CC(C(O)=O)=CC=C1	H _I N N YO	NCCNC(C)=O	° Contraction of the second se	OC(C1=CC=C(CCl)C=C1)=O	www.col	NCCC1=CC=C(OC)C(OC)=C1	HO ^L CO ^{CO}	CICC1=CC(C(0)=0)=CC=C1	
710	130224081609260317032810 2	HN	N1CCNCCC1	Lor.	CICC1-CC(C(0)-0)-CC-C1	HAN CON	NCC1-CC-CC(C(F)(F)F)-C1		CIC/C(C)=C/[C@@H](C)C(O)=O	www.col	NCCC1-CC-C(OC)C(OC)-C1	HO O S	oc([C@H](C)CI)−O.[S]	
688	130224071501260317022810 2	NH ₂	NCC1=CC=C(C)C=C1	ly-	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	www.cock	NCCC1=CC=C(OC)C(OC)=C1		CICC1=CC(C(O)=O)=CC=C1	
624	130224011502260617032810 2	H _L N B	NCC1=CC=CC(Br)=C1	l U	CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1	\mathcal{L}	OC(C1=CC=C(CCI)C=C1)=O	NUN COL	NCCC1=CC=C(OC)C(OC)=C1	HO O S	oc([C@H](C)CI)=O.[S]	
681	130224051504261017032810 2		NCC1=CC=C(OCO2)C2=C1	i de la come	CICC1=CC(C(O)=O)=CC=C1	H,M^Q	NCC1=CC=C(Cl)C=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	HAR COL	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]	
483	130124041503260617042810 2	NH ₂	NCC=C	он ОН	OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	° La Corre	OC(C1=CC=C(CCI)C=C1)=O	HAR COL	NCCC1=CC=C(OC)C(OC)=C1	HOLIGA	BrC1=CC=C(C(O)=O)C=C1	
468	130124031504260417022810 2	H ₂ N~0	NCCCOC	от сі	OC(C1=COC(CCI)=N1)=O	H,N~~H~	NCCNC(C)=O	° La Constantina de la Constan	OC(C1=CC=C(CCI)C=C1)=O		NCCC1=CC=C(OC)C(OC)=C1	He ^l toro	CICC1=CC(C(0)=0)=CC=C1	
517	130124071501260317012810 2	NH ₂	NCC1=CC=C(C)C=C1	OH CI	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	www.col	NCCC1=CC=C(OC)C(OC)=C1		OC(C1=CSC(CCI)=N1)=O	
584	130124091501260617022610 2	H.N~~~V_	NCCCN1C-CN-C1	CI OH	0C(C1-C0C(CCI)-N1)-0		N[C@@H](C)C1=CC=CC=C1	o=↓N OH	0C(C1=CSC(CCI)=N1)=0		NCCC1-CC-C(0C)C(0C)-C1	HO ^L CO ^{CO}	CICC1-CC(C(0)-0)-CC-C1	
591	130124091502260717032810 2	H.N~~V_	NCCCN1C=CN=C1	OH CI	OC(C1=COC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1	o= ↓ N OH	OC(C1=CSC(CCI)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]	
594	130124091504260417032810 2	~~~	NCCCN1C=CN=C1	Сн Сн	OC(C1=COC(CCI)=N1)=O	H'N~~H	NCCNC(C)=O	° La Constantina de la Const	OC(C1=CC=C(CCI)C=C1)=O	ward d	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]	
489	130124051501260917032810 2	**^^¢¢	NCC1=CC=C(OCO2)C2=C1	от сі он	OC(C1=COC(CCI)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	HUMAN CAL	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)CI)=0.[S]	
510	130124051510260417042810 2		NCC1=CC=C(OCO2)C2=C1	от сі он	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	····	CIC/C(C)=C/[C@@H](C)C(O)=O	HUN COL	NCCC1=CC=C(OC)C(OC)=C1	HOLING	BrC1=CC=C(C(O)=O)C=C1	
794	130324041503260917042810 2	MH ₂	NCC=C	СП С	OC(C1=CSC(CCI)=N1)=O	NA COL	NCC1=CC(F)=CC(C(F)(F)F)=C1	<pre></pre>	OC(C1=CSC(CCI)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1	HO	BrC1=CC=C(C(O)=O)C=C1	
823	130324071501260717032810 2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCl)=N1)=O	A Colores	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1	HO O S	0C([C@H](C)Cl)=0.[S]	
1111	131024031501200317042810 2	H ₂ N	NCC1=CC(F)=C(F)C=C1	K CI	OC(C1=C3C(CCl)=N1)=O	H ₂ N	NCC1=CC=C31	CI CI CH	OC(C1=COC(CCI)=N1)=O	www.co.	NCCC1=CC=C(OC)C(OC)=C1	HO	BrC1=CC=C(C(O)=O)C=C1	
1120	131024031502260417032810 2	H ₂ N	NCC1=CC(F)=C(F)C=C1	K CI CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N N YO	NCCNC(C)=O	°↓ CH	OC(C1=CC=C(CCl)C=C1)=O	www.co.	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)Cl)=O.[S]	
807	130324051501260817032810 2		NCC1=CC=C(OCO2)C2=C1	Сн Сн	OC(C1=CSC(CCI)=N1)=O	C NH,	N[C@@H](C)C1=CC=CC=C1	O= CH	OC(C1=CSC(CCI)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1	HO_O S	0C([C@H](C)Cl)=0.[S]	
923	130424041501260317012805 2	NH ₂	NCC=C	len'r o	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N.	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H,N	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O	
922	130424031510260417042805 2	H _I M	NCCCOC	l _{ri}	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	"	CIC/C(C)=C/[C@@H](C)C(O)=O	HIN	NCC1COC(C=CC=C2)=C2O1	HO O R	OC([C@H](C)Br)=O.[R]	

Section-10: Analysis of Naive bead population: These beads are deep sequenced after DEL synthesis (upto 2 copies) $\frac{1}{1} \frac{1}{1} \frac{1}{1} \frac{1}{2} \frac{1}{2} \frac{2}{2} \frac{2}{2} \frac{1}{2} \frac{1}{1} \frac$

					HO TO TO		H ₂ N		о-Сн		H ₂ N		s s	
2	130124071501260717022810	44	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	-horner	NCC1=CC=C(N(C)C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	N/ Co	NCCC1=CC=C(OC)C(OC)=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
3	130224031504260517032802	37	H ₂ N~0	NCCCOC	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O	ortica OH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
4	130224101503260317102804	37	HN	C1CNCCN1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1	o= oH	OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
5	130324041504260417092804	33	MH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	H ₂ N ^N ^H	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
6	130424071502260917032805	31	NH ₂	NCC1=CC=C(C)C=C1	HO LEAST	CIC/C(C)=C/(C@@H)(C)C(O)=O	wy Y	NOC1=CC(F)=OC(C(F)(F)F)=C1	o	OC(C1=CSC(CCI)=N1)=O		NCC1COC(C=CC=C2)=C2O1	HU S	OC([C@H](C)Cl)=O.[S]
7	130424061502260517032802	25	H ₂ N	NCC1=CC=CO1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
8	131024021502261017022809	23	H ₂ N	NCC1=CC(F)=C(F)C=C	HO ^L OCO	CICC1=CC(C(O)=O)=CC=C1	H,M C	NCC1=CC=C(CI)C=C1	······	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
9	130224091509260317032803	19	H ₂ N~~N^N	NCCCN1C=CN=C1	HO ²	CICC1=CC(C(O)=O)=CC=C1	with the	NCC1=CC=CC(C(F)(F)F)=C1	HOLINA	CIC/C(C)=C/(C@@H)(C)C(O)=O	H.M.~~YY	NCCCN1C=CN=C1	HO S	CC([C@H](C)Cl)=O.[S]
10	130124041509260317022804	18	MH ₂	NCC=C	O= OH	OC(C1=COC(CCI)=N1)=O	NA CA	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N	NCC1=CC=CO1	но	CICC1=CC(C(O)=O)=CC=
11	130924031509260217102804	18	Han	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	HAN CONT	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H2N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
12	130124071501260417102804	17	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N ^N ^H	NCCNC(C)=0	° ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	H2N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
13	130224031503260417092804	16	H2N~~~0~	NCCCOC	Ho ¹ CC a	CICC1=CC(C(O)=O)=CC=C1	H,N~~H~~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
14	131024021501260417102804	16	H ₂ N	NCC1=CC(F)=C(F)C=C	но	CICC1=CC(C(O)=O)=CC=C1	H,N N YO	NCCNC(C)=0	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
15	130124061509260117102804	15	H ₂ N	NCC1=CC=CO1		OC(C1=COC(CCI)=N1)=O	HAUNDY	NCC1=CC=CC(C(F)(F)F)=C1	····	CIC/C(C)=C/(C@@H)(C)C(O)=O	H,N S	N[C@@H](C)C1=CC=CC=C1.[S	o H	O=C(0)C1=C(C)OC=C1
16	130124071510260417032803	15	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HOLINA	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M~~N_V	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
17	130124101510260317092804	14	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	····ler	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
18	130224101510260317032803	14	HN	C1CNCCN1	HO ^L	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.~~NN	NCCCN1C=CN=C1	HO S	CC([C@H](C)Cl)=O.[S]
19	130224021501260417042806	13	H ₂ N	NCC1=CC=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H _w	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O R	CC([C@H](C)Br)=O.[R]
20	130124051502260417042803	12	HIN	NCC1=CC=C(OCO2)C:	OF OH	OC(C1=COC(CCI)=N1)=O	H _N N	NCCNC(C)=0	CH CI	OC(C1=CC=C(CCI)C=C1)=O	1.11~1 <u>~</u> 1_1	NCCCN1C=CN=C1	HO O R	CC([C@H](C)Br)=O.[R]
21	130124081502261017042803	12	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O	H _A N ^A CA	NCC1=CC=C(CI)C=C1	Hole Contraction	CIC/C(C)=C/[C@@H](C)C(O)=O	1,1/~ 1/ ₂ /1	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
22	130124081504260417102804	12	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O	н,w~~ ^Н ~°	NCCNC(C)=O	•↓ ₩	OC(C1=CC=C(CCI)C=C1)=O	H_N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(0)C1=C(C)OC=C1
23	130224031510260417092804	12	H ₂ N O	NCCCOC	но	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
24	130324101501260417022803	12	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H,N~~H~O	NCCNC(C)=0	° ↓ Û ^ °	OC(C1=CC=C(CCI)C=C1)=O	H,N~~N_)V	NCCCN1C=CN=C1	HO ^Î () (i	CICC1=CC(C(O)=O)=CC=
25	130424011503260517032802	12	H ₂ N Br	NCC1=CC=CC(Br)=C1	HO I TO A	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	CC([C@H](C)Cl)=O.[S]
26	130424031510260317032803	12	H ₂ N~0	NCCCOC	HO ^L Y ^A	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.~~NN	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
27	130124031504260417032803	11	H2N	NCCCOC		OC(C1=COC(CCI)=N1)=O	H _M N~H _Y O	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	1.11~~~Y_Y1	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
28	130424031504260817022803	11	H ₂ N~0~	NCCCOC	HO ^L Y ^Y	CIC/C(C)=C/[C@@H](C)C(O)=O	C NH2	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H,H ~ H_H	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=
29	130424031509260317092804	11	H ₂ N 0	NCCCOC	10 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	CIC/C(C)=C/[C@@H](C)C(O)=O	NA CY	NOC1=CC=CC(C(F)(F)F)=C1	m to the second	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	~О	CCC(0)=0
30	131024021501260217012808	11	H ₂ N	NCC1=CC(F)=C(F)C=C	HO	CICC1=CC(C(O)=O)=CC=C1	where the second s	NCC1=CC=C(S(=0)(C)=0)C=C	CI CI	OC(C1=COC(CCI)=N1)=O	H ₂ N	BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCI)=N1)=O
31	130124051502260417022804	10	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H2N ~~ ^H	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1	¹ 0^	CICC1=CC(C(O)=O)=CC=
32	130124051509260317032807	10	H ₂ N	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	······································	CIC/C(C)=C/[C@@H](C)C(O)=O	₹ Ţ	NCC1=CC(OC)=CC(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
33	130124071502260417092803	10		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H,N~~ ^H /O	NCCNC(C)=O	۰ ۳	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	HO. O S	OC([C@H](C)Cl)=0.[S]

34	130324031509260217102804	10		Amines(A1)-smiles		OC(C1=CSC(CCI)=N1)=O	H,H T	Amines(A2)-smiles NOC1=CC=CC(C(F)(F)F)=C1		ACI0(A2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ₄ s	N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
35	130324051503260117022803	10	H,N C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	H ₂ N 0	NCCOC		OC(C1=COC(CCI)=N1)=O	+++~~~V_+	NCCCN1C=CN=C1	новит	CICC1=CC(C(O)=O)=CC=
36	130324101502260217022803	10	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	***	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	HAN NON	NCCCN1C=CN=C1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=
37	130424051504260917022804	10	11,M~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(OCO2)C	OH Holy to a	CIC/C(C)=C/[C@@H](C)C(O)=O	**^Q	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	новорога	CICC1=CC(C(O)=O)=CC=
38	130124031502261017092803	9	H ₂ N	NCCCOC		OC(C1=COC(CCI)=N1)=O	H,N C	NOC1=CC=C(CI)C=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)Cl)=O.[S]
39	130124091501261017032802	9	ни	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H,N C	NOC1=CC=C(CI)C=C1	····ler	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N OH	NCCO	HU U S	OC([C@H](C)Cl)=O.[S]
40	130224101509260117102804	9	HN	C1CNCCN1	но Царана	CICC1=CC(C(O)=O)=CC=C1	w	NOC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	o H	O=C(O)C1=C(C)OC=C1
41	130324101510260317102804	9	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	····L	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N K	N(C@@H)(C)C1=CC=CC=C1.[S	o H	O=C(O)C1=C(C)OC=C1
42	130424031509260217032803	9	H ₂ N	NCCCOC	но	CIC/C(C)=C/[C@@H](C)C(O}=O	NA CAR	NOC1=CC=CC(C(F)(F)F)=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
43	130424081503260717032803	9		N1CONCCC1	····lysia	CIC/C(C)=C/[C@@H](C)C(O)=O	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HAI YO	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
44	130924031501260917032804	9	H ₂ N ⁻	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	HUN CON	NOC1=OC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=O.[S]
45	130924031504260417092804	9	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	H_N~H~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	~ ро	CCC(O)=O
46	130124031503260417092804	8	H ₂ N~~_0~	NCCCOC		OC(C1=COC(CCI)=N1)=O	H,N~H~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]	О ОН	CCC(O)=O
47	130124031504260817032809	8	H ₂ N	NCCCOC		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H _J N O	NCC1CCOCC1	HO C S	OC([C@H](C)CI)=O.[S]
48	130124051501261017102804	8	H _I N C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N C	NCC1=CC=C(CI)C=C1	ноците	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N S	N(C@@H)(C)C1=CC=CC=C1.[S	of the	0=C(0)C1=C(C)OC=C1
49	130124051503260617092804	8	H _N N	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
50	130124051509260317022803	8	H _I N C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	HAT ON	NCC1=CC=CC(C(F)(F)F)=C1	HO TOTAL	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
51	130224031502260817022802	8	H ₂ N~O	NCCCOC		CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO ^Î (jî ci	CICC1=CC(C(O)=O)=CC=
52	130224041504260717022803	8	NH ₂	NCC=C	HO ^L LJ ^{CO}	CICC1=CC(C(O)=O)=CC=C1	A CANING	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H.M.~~YY	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
53	130324071501260517102804	8		NCC1=CC=C(C)C=C1	<u> </u>	OC(C1=CSC(CCi)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	, CH	O=C(O)C1=C(C)OC=C1
54	130424031504260517032802	8	H ₂ N	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N /	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
55	130424031504260617032803	8	H2N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCOC	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	• 	OC(C1=CC=C(CCI)C=C1)=O	···~··	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
56	130424031504260917022809	8	H ₂ N O	NCCCOC		CIC/C(C)=C/(C@@H)(C)C(O)=O	HUN TO Y	NOC1=CC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
57	130424051502260417032803	8	H ₂ N CC	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N~ ^H ¢0	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H.N.~~N_)	NCCCN1C=CN=C1	HO C S	OC([C@H](C)CI)=O.[S]
58	130424071502260217022803	8		NCC1=CC=C(C)C=C1	HOLE AND	CIC/C(C)=C/[C@@H](C)C(O}=O	" Of	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	HAN NON	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
59	130424081509260317102804	8	HN	N1CONCCC1	····	CIC/C(C)=C/[C@@H](C)C(0)=O	HAR CON	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO A	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
60	130424091504260617022803	8	H _a n M _a n	NCCCN1C=CN=C1	HOLE TO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	of the second se	OC(C1=CC=C(CCI)C=C1)=0	H.M. ~ V.C.M	NCCCN1C=CN=C1	HOLOCA	CICC1=CC(C(O)=O)=CC=
61	130424101501260617032809	8	HN	C1CNCCN1	m lang	CIC/C(C)=C/[C@@H](C)C(0}=O		NCC1=CC=CC=C1	° ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)CI)=O.[S]
62	130124031502260217032803	7	H ₂ N~O	NCCCOC		0C(C1=C0C(CCI)=N1)=0	"	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H.M.~~YYM	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
63	130124071502260617092804	7	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	~Он	CCC(O)=O
64	130324051504260817032803	7		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NH,	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H.N.~~NN	NCCCN1C=CN=C1	HO CI S	OC([C@H](C)Cl)=O.[S]
65	130424031501261017022803	7	H ₂ N 0	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O	H _N	NCC1=CC=C(CI)C=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN TON	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
66	130424071502260317032805	7		NCC1=CC=C(C)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H,N	NCC1COC(C=CC=C2)=C2O1	HO. O S	OC([C@H](C)Cl)=0.[S]

observation 67	full.mol.code2 130424071509260417032803	copies 7	Amines(X1)	Amines(X1)-smiles NCC1=CC=C(C)C=C1	Acid(X1)	Acid(X1)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines(X2)	Amines(X2)-smiles NCC1=CC=CC(C(F)(F)F)=C1	Acid(X2)	Acid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines(X3)	Amines(X3)-smiles NCCCN1C=CN=C1	Structure of Pair	Pair3.Acids OC([C@H](C)Cl)=O.[S]
			NH ₂		Holy Co		HAN COX		HO		HAN NON		s s	
68	130424091502260317032803	7	ни	NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1	O= OH	OC(C1=COC(CCI)=N1)=O	HAI YON	NCCCN1C=CN=C1	s Development	OC([C@H](C)Cl)=O.[S]
69	130924031501260717042803	7	Han	NCCC1CCOCC1		OC(C1=CSC(CCi)=N1)=O	A CALINI	NCC1=CC=C(N(C)C)C=C1	Q= OH	OC(C1=CSC(CCI)=N1)=O	HAI YO	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
70	130924041501260417092804	7	HIN	NCCC1CCOCC1		CIC/C(C)=C/[C@@H](C)C(O)=O	H _M N	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H _J N	N[C@H](C)C1=CC=CC=C1.[R]	-~О ОН	CCC(O)=O
71	131024021503260417102804	7	H ₂ N	NCC1=CC(F)=C(F)C=C		CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H	NCCNC(C)=O	€ CH	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
72	130124031502261017032803	6	H ₂ N~0	NCCCOC	o=	OC(C1=COC(CCI)=N1)=O	H,N^C	NCC1=CC=C(CI)C=C1		CIC/C(C)=C/(C@@H)(C)C(O)=O	HAI ~ 101	NCCCN1C=CN=C1	HU U S	OC([C@H](C)Cl)=O.[S]
73	130124041501261017022803	6	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H _N N	NCC1=CC=C(CI)C=C1	HO I TO A	CIC/C(C)=C/[C@@H](C)C(O)=O	HW ~~ 104	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
74	130124051510260317032803	6	HĮN CON	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO TOTAL	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAI MON	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
75	130124071502260317092804	6		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
76	130124071504260217102804	6		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	***	NCC1=CC=C(S(=0)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
77	130224041501260517102804	6	MH ₂	NCC=C	no logo	CICC1=CC(C(O)=O)=CC=C1	H _a N	NCC(C)(C)O	° ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	othe othe	0=C(0)C1=C(C)0C=C1
78	130224081502260717032803	6	HN	N1CONCCC1	HO LOCA	CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	141 V	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=0.[S]
79	130224081503260417102804	6	HN	N1CONCCC1	NO CON	CICC1=CC(C(O)=O)=CC=C1	H_N~~H~~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
80	130324041502260417042803	6	MH ₂	NCC=C	OH CHART	OC(C1=CSC(CCI)=N1)=O	HJN~H~	NCCNC(C)=0	OF CI	OC(C1=CC=C(CCI)C=C1)=O	HAI YO	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
81	130324061503260417092804	6	H ₂ N	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O	H_N~~ ^H ~°	NCCNC(C)=0	۲ ۲ ۲ ۲	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	° Он	CCC(O)=O
82	130324081509260217102804	6	HN	N1CCNCCC1	Q → C → C → C → C → C → C → C → C → C →	OC(C1=CSC(CCI)=N1)=O	HAR OF Y	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO I	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
83	130424031502260217032803	6	H ₂ N~0	NCCCOC	HO TY O	CIC/C(C)=C/[C@@H](C)C(O)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C	O= OH	OC(C1=COC(CCI)=N1)=O	HAI ~ 10	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
84	130424031503260517092804	6	H ₂ N	NCCCOC	HOLINA	CIC/C{C}=C/[C@@H](C)C(0)=O	H ₂ N OH	NCC(C)(C)O	of the second se	0C(C1=CC=C(CCI)C=C1)=0	H _J N R	N[C@H](C)C1=CC=CC=C1.[R]	~ ↓ 0 ЮН	CCC(O)=O
85	130424051509260217092804	6	H _N	NCC1=CC=C(OCO2)C	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	NA CAN	NOC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	~Он	CCC(O)=O
86	130424101509260217022804	6	HN	C1CNCCN1	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O	with the second s	NOC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=
87	130924021501260317032803	6	H ₂ N	NCCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HAN MON	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
88	130924031502261017102804	6	Han	NCCC1CCOCC1		OC(C1=CSC(CCi)=N1)=O	H,N^C	NCC1=CC=C(CI)C=C1	HO I TATA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
89	130924031503261017032803	6	Han	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	HAN	NCC1=CC=C(CI)C=C1	₩ ^L ŧriγ~a	CIC/C(C)=C/[C@@H](C)C(O)=O	ни М	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
90	131024011504260617042809	6	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1	°↓↓↓ OH	0C(C1=CC=C(CCI)C=C1)=0	HJN	NCC1CCCCC1	HO CO R	OC([C@H](C)Br)=O.[R]
91	131024031504260517032802	6	H ₂ N	NCC1=CC(F)=C(F)C=C	O-OH	OC(C1=CSC(CCi)=N1)=O	H ₂ N /	NCC(C)(C)O	€ OH	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
92	130124051503261017042803	5	HĩN CHUN	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H _A N	NCC1=CC=C(CI)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HAI YO	NCCCN1C=CN=C1	HO O R	0C([C@H](C)Br)=0.[R]
93	130124051509260117012803	5	H _N	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN NON	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
94	130124051509260417032803	5	HIN CO	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	HAIL	NOC1=CC=CC(C(F)(F)F)=C1	₩ ^l trina	CIC/C(C)=C/[C@@H](C)C(O)=O	HANNA	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
95	130124071501260417032803	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H _N ~ ^H + ^o	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	HAI ~ YON	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
96	130124071501260617022803	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1	O CH	OC(C1=CC=C(CCI)C=C1)=O	141 ~~ 10 r	NCCCN1C=CN=C1	HOLICI	CICC1=CC(C(O)=O)=CC=
97	130124071501260817032804	5		NCC1=CC=C(C)C=C1	o tot	OC(C1=COC(CCI)=N1)=O	NH,	N[C@@H](C)C1=CC=CC=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H _a N	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=O.[S]
98	130124071501261017042803	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	HN	NCC1=CC=C(CI)C=C1	HOLING	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAI MON	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
99	130124071504260417102804	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N N Y O	NCCNC(C)=O	€ OH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1

100	130124071509260117022809	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	1	NCC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HO ^L	CICC1=CC(C(O)=O)=CC=
101	130124071509260417022803	5		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	HAR CONT	NCC1=CC=CC(C(F)(F)F)=C1	····land	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N~~Y_N	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
102	130124081502260417022809	5		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H ^H	NCCNC(C)=O	and the second s	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
103	130124091501260617022803	5	H2H ~~~ H_2H	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	ни ^{с~~~} чОч	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
104	130124091501260717032803	5	H,N ~ N _ N	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	A CANN	NOC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H,N~~N_N	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=0.[S]
105	130124091504260217022809	5	н,и~~ч_у	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	****	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(0)=0)=CC=
106	130124101502260417042803	5	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H ¢ ⁰	NCCNC(C)=0	OH of the second secon	OC(C1=CC=C(CCI)C=C1)=O	нистр	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
107	130124101503260417022803	5	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H _M	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	HUM NON	NCCCN1C=CN=C1	но	CICC1=CC(C(0)=0)=CC=
108	130224031502260717012803	5	H ₂ N	NCCCOC	OH HO ^L LLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLLL	CICC1=CC(C(O)=O)=CC=C1	A CLAM	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H.M.~~NN	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
109	130224031502260717032803	5	H ₂ N	NCCCOC		CICC1=CC(C(O)=O)=CC=C1	1. J. M.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H,II~~ II_)I	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=0.[S]
110	130224081510260317102804	5	HN	N1CONCCC1		CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N(C@@H)(C)C1=CC=CC=C1.[S	ot oth	O=C(O)C1=C(C)OC=C1
111	130224091504260617102804	5	н,и~~и_у	NCCCN1C=CN=C1	HO CON	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	oH oH	O=C(O)C1=C(C)OC=C1
112	130224101501260617012803	5		C1CNCCN1		CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
113	130224101502261017092804	5		C1CNCCN1	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H _M	NOC1=CC=C(CI)C=C1	···	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N(C@H)(C)C1=CC=CC=C1.[R]		CCC(O)=O
114	130224101509260317032803	5	HN	C1CNCCN1	HO CO	CICC1=CC(C(O)=O)=CC=C1	HALL	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	S	0C([C@H](C)Cl)=0.[S]
115	130324031503260417022803	5	H ₂ N	NCCCOC	Jan a	OC(C1=CSC(CCI)=N1)=O	H,N~H	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H,M M	NCCCN1C=CN=C1	ноцит	CICC1=CC(C(O)=O)=CC=
116	130324041509260317022804	5	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	HAN CON	NOC1=CC=CC(C(F)(F)F)=C1	m lang	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	но	CICC1=CC(C(O)=O)=CC=
117	130324051502261017042803	5	H _A N ()	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	HAN	NCC1=CC=C(Cl)C=C1	m to the second	CIC/C(C)=C/[C@@H](C)C(O)=O	HUN - MON	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
118	130324051504260817012803	5	H _N CC	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H,M~~NM	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
119	130324051509260417042803	5	H,N	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NUT Y	NOC1=CC=CC(C(F)(F)F)=C1	HOL IN	CIC/C(C)=C/[C@@H](C)C(O)=O	1.11~1 ₀ 1	NCCCN1C=CN=C1	HO CH R	OC([C@H](C)Br)=O.[R]
120	130324071503261017022803	5	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	HANCO	NCC1=CC=C(CI)C=C1	Holen to	CIC/C(C)=C/[C@@H](C)C(O)=O	1.11~~N_)1	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
121	130324091510260317032803	5	H,H ~ Y _ Y	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HO I TO TO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	HO S	0C([C@H](C)Cl)=0.[S]
122	130324101502260417032801	5	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H,N~~H	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	Bat	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)Cl)=0.[S]
123	130324101503260417022803	5		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H _N ~ ^H + ⁰	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H.H.~~~YH	NCCCN1C=CN=C1	HO ^Î () a	CICC1=CC(C(O)=O)=CC=
124	130424031502260317032809	5	H ₂ N~0~	NCCCOC		CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=O.[S]
125	130424031502260417022805	5	H ₂ N~0~	NCCCOC	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HJN~H	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	HUN	NCC1COC(C=CC=C2)=C2O1	HO ^Î () ^a	CICC1=CC(C(O)=O)=CC=
126	130424031504260417102803	5	H ₂ N~0	NCCCOC	In the second	CIC/C(C)=C/[C@@H](C)C(O)=O	HĮN H	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	HO S	OC([C@H](C)Cl)=0.[S]
127	130424031504260617032809	5	H ₂ N~~_0~	NECCOC	HO TOTA	CIC/C(C)=C/[C@@H](C)C(0)=0		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO S	0C([C@H](C)Cl)=0.[S]
128	130424051504261017102804	5	HAN	NCC1=CC=C(OCO2)C	notro	CIC/C(C)=C/[C@@H](C)C(O)=O	HW	NCC1=CC=C(CI)C=C1	m land	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	oH o	O=C(O)C1=C(C)OC=C1
129	130424091502260217032802	5	н,и~~и_у	NCCCN1C=CN=C1	Holy o	CIC/C(C)=C/[C@@H](C)C(O)=O	***	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
130	130424091502260817032803	5	н,п~~пп	NCCCN1C=CN=C1	₩ [°] ₽ [~]	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HJN~~N	NCCCN1C=CN=C1	HO O S	0C([C@H](C)Cl)=0.[S]
131	130424101504260317032803	5	HN	C1CNCCN1	no la proposition	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H,M~~N_N	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
132	130924021509260417022803	5	H _M	NCCC1CCOCC1	HO	CICC1=CC(C(O)=O)=CC=C1	NUN Y	NCC1=CC=CC(C(F)(F)F)=C1	HO LA CH	CIC/C(C)=C/[C@@H](C)C(O)=O	HUN NON	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=

133	130924031501260217032809	5	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCl)=N1)=O	***	NCC1=CC=C(S(=O)(C)=O)C=C	CH CI	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=O.[S]
134	131024021501261017102804	5	HaN	NCC1=CC(F)=C(F)C=C	·	CICC1=CC(C(O)=O)=CC=C1	HAN CO	NOC1=CC=C(Cl)C=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H _J N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
135	131024021502260617102804	5	H ₂ N F	NCC1=CC(F)=C(F)C=0	Hologra	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		0C(C1=CC=C(CCI)C=C1)=0	H _J N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
136	130124021509260317102804	4	H ₂ N	NCC1=CC=CN=C1		OC(C1=COC(CCI)=N1)=O	with the second se	NCC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	HJN S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
137	130124031504260517032802	4	H ₂ N	NCCCOC	Q Q OH OH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	OH CON	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
138	130124031509260117032810	4	H ₂ N O	NCCCOC	O	OC(C1=COC(CCI)=N1)=O	нистр	NCC1=CC=CC(C(F)(F)F)=C1	no la francia	CIC/C(C)=C/(C@@H)(C)C(O)=O	RUN COL	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
139	130124041502260417032803	4	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N N YO	NCCNC(C)=0		0C(C1=CC=C(CCI)C=C1)=0	HM NON	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
140	130124041504260517032802	4	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	ortice OH	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
141	130124041510260217032803	4	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HOLING	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAI ~ 10	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
142	130124051501260417032801	4	H _k N C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H _J N~ ^H Y ⁰	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	HUN	NCCC1=CNC2=OC=CC=C21	HO S	OC([C@H](C)Cl)=O.[S]
143	130124051501260817032804	4	H,N C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=O.[S]
144	130124051502260417032803	4	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H _A N ^H ^Y	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H,M ~ NCM	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
145	130124051502260517102804	4	H ₂ M 0	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	•↓ OH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
146	130124051502260817042809	4	H _k N	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	Real Provided International Provided Internat	N[C@@H](C)C1=CC=CC=C1	CI CI	OC(C1=CSC(CCI)=N1)=O	HUN	NCC1CCOCC1	HO O Br R	OC([C@H](C)Br)=O.[R]
147	130124051503260817022802	4	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	C NH2	N[C@@H](C)C1=CC=CC=C1	C → C → C → C → C → C → C → C → C → C →	OC(C1=CSC(CCI)=N1)=0	H ₂ N OH	NCCO	HO LOCA	CICC1=CC(C(O)=O)=CC=
148	130124051504260317042803	4	H _k N	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	CI C	OC(C1=COC(CCI)=N1)=O	HAI YO	NCCON1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
149	130124051504260517032802	4	H ₂ N C C O	NCC1=CC=C(OCO2)C	o=↓ OH	OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	o _↓ ↓ OH	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
150	130124051504260817032804	4	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	Killer (N[C@@H](C)C1=CC=CC=C1	CI CI CI	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=0.[S]
151	130124051509260217022803	4	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	NAL CAR	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN NON	NCCCN1C=CN=C1	HO	CICC1=CC(C(O)=O)=CC=
152	130124071501260817042803	4	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	Real Real Provide Action of the second secon	N[C@@H](C)C1=CC=CC=C1	OH CI	OC(C1=CSC(CCI)=N1)=O	HAN NN	NCCON1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
153	130124071501261017032804	4	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H _A N CO	NCC1=CC=C(CI)C=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)CI)=O.[S]
154	130124071502260317032803	4	NH ₂	NCC1=CC=C(C)C=C1	o= OH OH	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	O OH OH	OC(C1=COC(CCi)=N1)=O		NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
155	130124071503260317032803	4	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	OF OH	OC(C1=COC(CCI)=N1)=O	HAN MON	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
156	130124071503260717012803	4	NH ₂	NCC1=CC=C(C)C=C1	O-CH	OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1	OH CI	OC(C1=CSC(CCI)=N1)=O	ни	NCCCN1C=CN=C1	O-OH	OC(C1=CSC(CCI)=N1)=O
157	130124071504260917022803	4	NH ₂	NCC1=CC=C(C)C=C1	o → OH OH	OC(C1=COC(CCI)=N1)=O	nu qt	NCC1=CC(F)=CC(C(F)(F)F)=C1	CH CI	OC(C1=CSC(CCI)=N1)=O	ни	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
158	130124071504260917042803	4	NH ₂	NCC1=CC=C(C)C=C1	O-CH	OC(C1=COC(CCI)=N1)=O	NA COL	NCC1=CC(F)=CC(C(F)(F)F)=C1	OH CI	OC(C1=CSC(CCI)=N1)=O	HANNA	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
159	130124071509260417102804	4	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NUT C	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
160	130124081502260217012803	4	HN	N1CONCCC1	o= OH	OC(C1=COC(CCI)=N1)=O		NCC1=CC=C(S(=0)(C)=0)C=C	OF OH	OC(C1=COC(CCI)=N1)=O	HN NO	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
161	130124081502261017012810	4	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O	H _A N C	NCC1=CC=C(CI)C=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	nur al	NCCC1=CC=C(OC)C(OC)=C1	S CI S CI OH	OC(C1=CSC(CCI)=N1)=O
162	130124081509260117102804	4	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O	HALL I	NCC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
163	130124091502260617032804	4	н,м	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H _a N	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=0.[S]
164	130124091503260617092804	4	H2N NCN	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
165	130224031501260417032804	4	H ₂ N~0	NCCCOC	HO CO	CICC1=CC(C(O)=O)=CC=C1	H _N	NCCNC(C)=0	of the second se	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCC1=CC=CO1	HO. JO S	0C([C@H](C)Cl)=0.[S]

observation 166	full.mol.code2 130224031502260717012809	4	Amines(X1) Amines(X1)-smiles	Adid(X1)	Acid(X1)-smiles Amines(X2) CICC1=CC(C(O)=O)=CC=C1	Amines(X2)-smiles Acid(X2 NCC1=CC=C(N(C)C)C=C1	CI OC(C1=CSC(CCI)=N1)=O	Amines(X3)	Amines(X3)-smiles NCC1CCOCC1	Structure of Pair	Pair3.Acids OC(C1=CSC(CCI)=N1)=O
167	130224031504260617032803	4	NCCCOC		CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC=C1	CI OC(C1=CC=C(CCI)C=C1)=0		NCCCN1C=CN=C1	о= он ноs	OC([C@H](C)Cl)=O.[S]
168	130224051501260217022803	4	H,N 0	lun line	CICC1=CC(C(O)=O)=CC=C1	NCC1=CC=C(S(=O)(C)=O)C=C ⁺	CI OC(C1=COC(CCI)=N1)=O	H,N~~ 10 M	NCCCN1C=CN=C1	×0 	CICC1=CC(C(0)=0)=CC=
169	130224051501260417102801	4	NCC1=CC=C(OCO2)C		CICC1=CC(C(0)=0)=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	H,N	N[C@@H](C)C1=CC=CC=C1.[S	$\sum_{i=1}^{i}$	OC(C1=CSC(CCI)=N1)=O
170	130224071501260217032801	4	NCC1=CC=C(C)C=C1	· · · · · · · · · · · · · · · · · · ·	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=C(S(=0)(C)=0)C=C N	CI OC(C1=COC(CCI)=N1)=O	R	NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=0.[S]
171	130224071501260617042803	4	NCC1=CC=C(C)C=C1	······································	CICC1=CC(C(0)=0)=CC=C1	NOC1=CC=CC=C1			NCCCN1C=CN=C1		OC([C@H](C)Br)=0.[R]
172	130224071502260317042803	4	NCC1=CC=C(C)C=C1	· ·	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CS1	CI 0C(C1=C0C(CCi)=N1)=0	HN 100	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
173	130224071503260317032809	4	NCC1=CC=C(C)C=C1	, in the second		NCC1=CC=CS1	CI OC(C1=COC(CCI)=N1)=0		NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=0.[S]
174	130224071509260417102803	4	NCC1=CC=C(C)C=C1	in the second	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	HO S	OC([C@H](C)CI)=O.[S]
175	130224081504260317032803	4			CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=CS1	CI 0C(C1=C0C(CCI)=N1)=0		NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
176	130224081510260417102804	4		· ·		CC(C)CCN	CIC/C(C)=C/[C@@H](C)C(O)=O	Hyll	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
177	130224091504260417092804	4		, in the second			OC(C1=CC=C(OCI)C=C1)=0	H ₂ N K	N[C@H](C)C1=CC=CC=C1.[R]		CCC(0)=0
178	130224091504260817012803	4		····	CICC1=CC(C(O)=O)=CC=C1	ын N[C@@H](C)C1=CC=CC=C1	C OC(C1=CSC(CCI)=N1)=0		NCCCN1C=CN=C1	OH	OC(C1=CSC(CCI)=N1)=O
179	130224091509260317032804	4		HO ^Î reșta	CICC1=CC(C(O)=O)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1		OC([C@H](C)Cl)=0.[S]
180	130224091510260317022803	4		HO ²		CC(C)CCN	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCON1C=CN=C1		CICC1=CC(C(O)=O)=CC=
181	130224101501260417022810	4		HO ^Î rena d			CI OC(C1=CC=C(CCI)C=C1)=0	. Ad	NCCC1=CC=C(OC)C(OC)=C1	₩ ¹	CICC1=CC(C(O)=O)=CC=
182	130224101501260717092804	4		HO ²	CICC1=CC(C(O)=O)=CC=C1	NCC1=CC=C(N(C)C)C=C1	C OC(C1=CSC(CCI)=N1)=0	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	\sim	CCC(O)=O
183	130224101502260417092802	4		HO ^Î rena d			CI OC(C1=CC=C(CCI)C=C1)=0	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	он	CICC1=CC(C(O)=O)=CC=
184	130224101502260517102804	4		IND THE REAL PROPERTY OF	CICC1=CC(C(O)=O)=CC=C1		CI OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	J OH	O=C(O)C1=C(C)OC=C1
185	130224101503260517102804	4		بر المراجع	CICC1=CC(C(O)=O)=CC=C1		CI OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	, CH	O=C(O)C1=C(C)OC=C1
186	130224101503261017102804	4		HO ^L YYO	CICC1=CC(C(0)=0)=CC=C1	NCC1=CC=C(CI)C=C1	CIC/C(C)=C/[C@@H](C)C(O)=O	H2N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
187	130224101504260817032805	4		"	CICC1=CC(C(0)=0)=CC=C1	N[C@@H](C)C1=CC=CC=C1	CI OC(C1=CSC(CCI)=N1)=0	H ₂ N ^A	NCC1COC(C=CC=C2)=C2O1	HO_O_S	OC([C@H](C)Cl)=0.[S]
188	130224101509260117032801	4		HO ^L Y O	CICC1=CC(C(O)=O)=CC=C1	NCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/[C@@H](C)C(O)=O	. 8.	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=0.[S]
189	130224101510260417022803	4		بر ساریک	CICC1=CC(C(O)=O)=CC=C1		CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	HI CON	CICC1=CC(C(O)=O)=CC=
190	130224101510260417032803	4		HO ^L LJ ^{CO}	CICC1=CC(C(0)=0)=CC=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	нистр	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
191	130324031501260417102803	4	HJN VCCCOC	<u> </u>	OC(C1=CSC(CCI)=N1)=O		CI OC(C1=CC=C(CCI)C=C1)=0	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)Cl)=O.[S]
192	130324031501260717032803	4	HJN 0		0C(C1=CSC(CCI)=N1)=0		CI OC(C1=CSC(CCI)=N1)=O		NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
193	130324031509260417032803	4	HJN 0 NCCCOC		0C(C1=CSC(CCI)=N1)=0	NCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/[C@@H](C)C(O)=O	1,11~~~1 ₂)1	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
194	130324041502260217032803	4	NCC=C		OC(C1=CSC(CCI)=N1)=O	NCC1=CC=C(S(=0)(C)=0)C=C ⁺	CI 0C(C1=C0C(CCI)=N1)=0	H,N~~NN	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
195	130324051501260417032806	4	H,N ~ () NCC1=CC=C(0C02)C		0C(C1=CSC(CCI)=N1)=0	NCCNC(C)=0	CI 0C(C1=CC=C(0CI)C=C1)=0	$\hat{\mathbf{Q}}$	NC[C@H](C)C1=CC=CC=C1	HOLOS	0C([C@H](C)CI)=0.[S]
196	130324051509260117032803	4	H,N (0002)C		0C(C1=CSC(CCl)=N1)=0	NCC1=CC=CC(C(F)(F)F)=C1	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N NO	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
197	130324051510260417032809	4	H_N NCC1=CC=C(OCC02)C		OC(C1=CSC(CCI)=N1)=O		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=O.[S]
198	130324071504260517032802	4	NCC1=CC=C(C)C=C1		DC(C1=CSC(CCI)=N1)=0	NCC(C)(C)O	\[\colored{c}_{c1} \] OC(C1=CC=C(CCI)C=C1)=0 \]	H ₂ N OH	NCCO	HOOS	0C([C@H](C)Cl)=0.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair	Pair3.Acids
199	130324081502260617022803	4	HN	N1CONCCC1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	€ CH	OC(C1=CC=C(CCI)C=C1)=0	HV/~_V_V	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
200	130324081509260117092804	4	HN	N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	····len	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]	~О	CCC(O)=O
201	130324091504260217032803	4	нли	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	***	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	HALLON	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
202	130324101502260417102804	4	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H _M N~ ^H + ^D	NCCNC(C)=0	e tan	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
203	130324101504261017032803	4	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H _A N^Q_C	NCC1=CC=C(CI)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HUM 101	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)Cl)=0.[S]
205	130424031502260617012809	4	H ₂ N~0	NCCCOC	no la presiona	CIC/C(C)=C/(C@@H)(C)C(O)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
206	130424031504260617032805	4	H ₂ N~0	NCCCOC	no la presiona	CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	HuN	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=O.[S]
207	130424041502260517032805	4	MH ₂	NCC=C	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	HIN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=O.[S]
208	130424041503260717102804	4	MH ₂	NCC=C	HOLING	СІС/С(С)=С/[С@@H](С)С(0)=0	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=0	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
209	130424051501260517092804	4	HIN	NCC1=CC=C(OCO2)C	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC(C)(C)O	€ CH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[O@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
210	130424051504280517032802	4	H _N C	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	H _a N	NCC(C)(C)O	°↓ OH	OC(C1=CC=C(CCI)C=C1)=O	H _z N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
211	130424051509260217032805	4	HAN	NCC1=CC=C(OCO2)C	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAN CONT	NCC1=CC=CC(C(F)(F)F)=C1	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	HJN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=O.[S]
212	130424071501260617022809	4	NH ₂	NCC1=CC=C(C)C=C1	no la porto	CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC=CC=C1	°↓ () ()	OC(C1=CC=C(OCI)C=C1)=O	H _L N	NCC1CCOCC1	HO ^L	CICC1=CC(C(O)=O)=CC=
213	130424071509260217032802	4	NH ₂	NCC1=CC=C(C)C=C1	₩ ^L ŧ	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN CON	NOC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
214	130424091501260317032803	4	н,п	NCCCN1C=CN=C1	HO TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	"" "D"	NCCCN1C=CN=C1	S S	OC([C@H](C)Cl)=O.[S]
215	130424091501260417032803	4	ним	NCCCN1C=CN=C1	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N~~H~	NCCNC(C)=0	o toto	OC(C1=CC=C(CCI)C=C1)=0	HA	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=0.[S]
216	130424091504260517102804	4	ним	NCCCN1C=CN=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	° ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(OCI)C=C1)=0	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	othe othe othe othe othe othe othe othe	O=C(O)C1=C(C)OC=C1
217	130424091504261017022803	4	н,н	NCCCN1C=CN=C1	HOLINA	CIC/C(C)=C/[C@@H](C)C(O)=O	HÌN	NCC1=CC=C(CI)C=C1	Holy of	CIC/C(C)=C/[C@@H](C)C(O)=O	HA	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(0)=0)=CC=
218	130424091509260217022803	4	H,N N N	NCCCN1C=CN=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	w	NCC1=CC=CC(C(F)(F)F)=C1	HO TOTAL	CIC/C(C)=C/[C@@H](C)C(O)=O	""~~D"	NCCON1C=CN=C1	HO ^L	CICC1=CC(C(0)=0)=CC=
219	130424101502260217022803	4	HN	C1CNCCN1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	"" "	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
220	130424101502260817022804	4	HN	C1CNCCN1		CIC/C(C)=C/[C@@H](C)C(O)=O	Real Provided Action of the second se	N[C@@H](C)C1=CC=CC=C1	o= OH	OC(C1=CSC(CCI)=N1)=0	H ₂ N	NCC1=CC=CO1	Ho ¹	CICC1=CC(C(O)=O)=CC=
221	130424101502261017022807	4	HN	C1CNCCN1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N^C	NCC1=CC=C(Cl)C=C1	HO I I I I I I I I I I I I I I I I I I I	CIC/C(C)=C/[C@@H](C)C(O)=O	₹¶.	NCC1=CC(OC)=CC(OC)=C1	ю ⁻¹ -0а	CICC1=CC(C(O)=O)=CC=
222	131024021502260417092804	4	HaN	NCC1=CC(F)=C(F)C=C	"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H Y ^O	NCCNC(C)=0	°↓ OH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
223	131024031501260417032810	4	H _a N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H,N N	NCCNC(C)=0	€ OH	OC(C1=CC=C(OCI)C=C1)=O	RAN CON	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)CI)=O.[S]
224	131024031503260317032806	4	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		oc(C1=COC(CCI)=N1)=0	NH ₂	NC[0@H](C)C1=CC=CC=C1	HO O S	0C([C@H](C)CI)=0.[S]
225	131024031503260417032804	4	Han	NCC1=CC(F)=C(F)C=C	OF OH	OC(C1=CSC(CCI)=N1)=O	H,N H	NCCNC(C)=O	€ OH	oc(c1=cc=c(ccl)c=c1)=o	H ₂ N O	NCC1=CC=CO1	HO O S	oc([c@H](c)cl)=0.[S]
226	131024031503260417042803	4	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H _A N~ ^H Y ⁰	NCCNC(C)=0	€ CH	oc(c1=cc=c(cci)c=c1)=o	"" "D'	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
221	131024031504250817032810	4	Han	NCC1=CC(F)=C(F)C=C	OH CH	0C(C1=CSC(0C)=N1)=0	NH ₂	NICEBHIC)C1=CC=CC=C1		00(C1=CS0(CCI)=N1)=0	RJW~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCC1=CC=C(CC)C(CC)=C1	HO CO S	ос([с@н](с)с)≡0.[s]
228	130124011502260917092802	3	H ₂ N	NCC1=CC=CC(Br)=C1	<pre></pre>	OC(C1=COC(CCI)=N1)=O	wyt	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=0	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO ^Î () a	CICC1=CC(C(0)=0)=CC=
220	130124021502260317032803	3	H ₂ N N	NGCIEGGEGNECT	O=OH		H ₂ N S	NCO18001 2			HA		HO CO S	00000-2
230	130124031501260417092804	3		NCCCOC	OF OH	00(01=000(001)=N1)=0	H ₂ N ^H TO	N004-00-004		00(01-000/001-141 2	H,N T n	NCCC1-CC-CCC2C1.[R]	ОН	
222	130124031802200317032810	3	H ₂ N	NCCCOC	O=OH	00(01=000(001=111=0	H ₂ N	NO01=00=08101000=01		00(01=000(001)=111=0	HUN-CO	NCCCNIC=C0=C(UC)C(UC)=C1	HO O S	000000000000000000000000000000000000000
232	137124031302260717032803	3	H ₂ N	NULLUC	O= OH	00(C1=00C(CCI)=N1)=0	A CALINA	NUCT=UC=U(N(U)C)C=C1		~~(CG)=N1)=0	HALL DI	NUCUNIC=CN=C1	HO. O S	~~[∪@H](C)CI)=0.[S]

233	130124031503260817032801	3	H ₂ N~O	NCCCOC		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ H	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=O.[S]
234	130124031503260917032803	3	H ₃ N	NCCCOC	o= OH	OC(C1=COC(CCI)=N1)=O	HAR CON	NOC1=CC(F)=OC(C(F)(F)F)=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	HN~~NON	NCCCN1C=CN=C1	HO C S	OC([C@H](C)Cl)=O.[S]
235	130124031509260217012809	3	H ₂ N~0~	NCCCOC		OC(C1=COC(CCI)=N1)=O	with the second s	NOC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
236	130124041501261017022809	3	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	HyM CO.	NCC1=CC=C(CI)C=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
237	130124041501261017042803	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	HAN	NCC1=CC=C(CI)C=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	··/~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
238	130124041502260417102803	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H ^A	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	HANK S	N[C@@H](C)C1=CC=CC=C1.[S	HU U S	OC([C@H](C)Cl)=O.[S]
239	130124041504260417032804	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H ^A	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=O.[S]
240	130124041504260417092804	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H _J N N YO	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	~О	CCC(O)=0
241	130124041510260317102803	3	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H2N S	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)CI)=O.[S]
242	130124051501260317032802	3	HAN	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
243	130124051501260917022805	3	H ₂ N C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	wyt	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H _A N	NCC1COC(C=CC=C2)=C2O1	но	CICC1=CC(C(O)=O)=CC=
244	130124051502260317022803	3	H,N CC	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	"" "	NCCCN1C=CN=C1	HO ^Î () ()	CICC1=CC(C(O)=O)=CC=
245	130124051502260417012804	3	H ₂ N	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H_N~~H~~~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	II2N O	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
246	130124051503260417012808	3	HIN CO	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H,N~H~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H _A N Constant	BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCI)=N1)=O
247	130124051503260417032806	3	H,N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H,N~~H~O	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	S	OC([C@H](C)CI)=O.[S]
248	130124051503261017012809	3	H _A N CC	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	HAN	NCC1=CC=C(CI)C=C1	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
249	130124051504260817032809	3	HJN CO	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)CI)=O.[S]
250	130124051504260917012809	3	H ₂ N CC	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	HAR OF Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
251	130124061510260317102804	3	H ₂ N	NCC1=CC=CO1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
252	130124071501260117102804	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N O	NCCOC	C CI	OC(C1=COC(CCI)=N1)=0	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	of the	O=C(O)C1=C(C)OC=C1
253	130124071501260417022803	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H,N~H~O	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	HUM NO1	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
254	130124071501260617032801	3	NH,	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H,M	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)Cl)=O.[S]
255	130124071501260717012809	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1	OH CI	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CC0CC1		OC(C1=CSC(CCI)=N1)=O
256	130124071501260817032803	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	Real Provided International Provided Internat	N[C@@H](C)C1=CC=CC=C1	CH CI	OC(C1=CSC(CCI)=N1)=O	HAIL 10	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
257	130124071501260817032809	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	C NH ₂	N[C@@H](C)C1=CC=CC=C1	CI C	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=O.[S]
258	130124071501260917092804	3	NH ₂	NCC1=CC=C(C)C=C1	OF OH	OC(C1=COC(CCI)=N1)=O	HAR OF Y	NOC1=CC(F)=OC(C(F)(F)F)=C1	OH CI	OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
259	130124071502261017022808	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	HAN	NCC1=CC=C(CI)C=C1	Ho Land	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N C	BrC1=CC=C(CN)C=C1	но	CICC1=CC(C(0)=0)=CC=
260	130124071502261017092804	3	NH ₂	NCC1=CC=C(C)C=C1	o=↓ OH	OC(C1=COC(CCI)=N1)=O	HŴ	NOC1=CC=C(CI)C=C1	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
261	130124071503260617032802	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NOC1=CC=CC=C1	•↓↓↓↓↓	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
262	130124071504260517032802	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	OF CH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
263	130124071504260617022804	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H _a N	NCC1=CC=CO1	"i_{0~}	CICC1=CC(C(O)=O)=CC=
264	130124071509260117102803	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	with the	NCC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	HO S	OC([C@H](C)CI)=O.[S]
265	130124081501260217022803	3		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(OCI)=N1)=O	"" "D"	NCCCN1C=CN=C1	HO	CICC1=CC(C(O)=O)=CC=

266	130124081501260217032802	3		NICONCCC1		OC(C1=COC(CCI)=N1)=O	HAN COR	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO		OC([C@H](C)Cl)=0.[S]
267	130124081501260517032805	3	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	HAN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=0.[S]
268	130124081502261017012809	3	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O	H _A N C	NCC1=CC=C(CI)C=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
269	130124081503260517022809	3		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCC1CCOCC1	HO ^L CO ^{CO}	CICC1=CC(C(O)=O)=CC=
270	130124081503260517092804	3		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	~ ро	CCC(O)=O
271	130124081509260317042803	3		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	ни	NCC1=CC=CC(C(F)(F)F)=C1	no la porto	CIC/C(C)=C/(C@@H)(C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	HU U R	OC([C@H](C)Br)=O.[R]
272	130124091501260517092802	3	H ₂ H N	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	новит	CICC1=CC(C(O)=O)=CC=
273	130124091501260617042803	3	H ₂ N N	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
274	130124091502260317022809	3	ни	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	новит	CICC1=CC(C(0)=0)=CC=
275	130124091502260417042803	3	H ₂ H	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	HJN~H~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H,N~~N_ON	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
276	130124091502260717092804	3	ни	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	О	CCC(O)=O
277	130124091502260917022809	3	ни	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	w	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HIN	NCC1CCOCC1		CICC1=CC(C(O)=O)=CC=
278	130124091503260517032803	3	020~~~n_n_N	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	···~~	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=0.[S]
279	130124091504260517022803	3	н_п	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC(C)(C)O	e to the second	OC(C1=CC=C(CCI)C=C1)=O	HANCON	NCCCN1C=CN=C1	но	CICC1=CC(C(0)=0)=CC=
280	130124091504260917042803	3	н"п~~п~л	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	HALL OF	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H.M.~~N_OH	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
281	130124091509260217032803	3	н_п	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	NA CA	NOC1=CC=CC(C(F)(F)F)=C1	m land	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN NON	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=0.[S]
282	130124091509260317022804	3	ним	NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O	nu t	NOC1=CC=CC(C(F)(F)F)=C1	····	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1	но	CICC1=CC(C(0)=0)=CC=
283	130124101503260717032803	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	····	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
284	130124101503260717102804	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
285	130124101503260817032803	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	1,01~10)	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
286	130124101503260817042803	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	C NH,	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HUN - MC/H	NCCCN1C=CN=C1	HO CO R	OC([C@H](C)Br)=O.[R]
287	130124101504260617032803	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	······································	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
288	130124101504261017012805	3	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	HAN	NOC1=CC=C(CI)C=C1	····l	CIC/C(C)=C/[C@@H](C)C(O)=O	Han	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
289	130224011503260717032803	3	H ₂ N	NCC1=CC=CC(Br)=C1		CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HUI NO	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)Cl)=O.[S]
290	130224011504260817032809	3	H ₂ N Br	NCC1=CC=CC(Br)=C1	HO ^L CCC a	CICC1=CC(C(O)=O)=CC=C1	C NH2	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=0.[S]
291	130224031501260417022809	3	H ₂ N O	NCCCOC	HOLOCA	CICC1=CC(C(O)=O)=CC=C1	H _J N ^H ^O	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(0)=0)=CC=
292	130224031501260617022805	3	H ₂ N~O	NCCCOC		CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	Hall	NCC1COC(C=CC=C2)=C2O1	Ho ¹ Co	CICC1=CC(C(O)=O)=CC=
293	130224031503260817102804	3	H ₂ N 0	NCCCOC		CICC1=CC(C(O)=O)=CC=C1	NH.	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
294	130224031504260817032803	3	H ₂ N~O	NCCCOC	HO ^L OTO	CICC1=CC(C(O)=O)=CC=C1	P.NH.	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H,N~~N_DN	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
295	130224031504261017012803	3	H ₂ N~~_0~	NCCCOC		CICC1=CC(C(O)=O)=CC=C1	HAN	NCC1=CC=C(CI)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	1,1~~~1Q1	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
296	130224031509260417032810	3	112N~~0~	NCCCOC	<u> </u>	CICC1=CC(C(O)=O)=CC=C1	~~~~`X'	NCC1=CC=CC(C(F)(F)F)=C1	₩ [°] ₽ ⁴ ~°	CIC/C(C)=C/[C@@H](C)C(O)=O	NUT CO	NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=O.[S]
297	130224041504260417092804	3	NH ₂	NCC=C		CICC1=CC(C(O)=O)=CC=C1	H_N N	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	~ рон	CCC(O)=O
298	130224041509260217092804	3	NH ₂	NCC=C	HOLOCA	CICC1=CC(C(O)=O)=CC=C1	HUNDY.	NCC1=CC=CC(C(F)(F)F)=C1	m into	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O

299	130224041509260417032803	3	Amines(X1)	Amines(X1)-smiles NCC=C		Acid(X1)-smiles CICC1=CC(C(O)=O)=CC=C1		Amines(X2)-smiles NOC1=CC=CC(C(F)(F)F)=C1		Acid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O		Amines(X3)-smiles NCCCN1C=CN=C1	HO S	Pair3.Acids OC([C@H](C)Cl)=O.[S]
300	130224051501260517022803	3	HJN CCC	NCC1=CC=C(OCO2)C	**************************************	CICC1=CC(C(O)=O)=CC=C1	H ₂ N H	NCC(C)(C)O	o _↓ ,) ∩ (I	OC(C1=CC=C(CCI)C=C1)=O	HAI~~YON	NCCCN1C=CN=C1	HO ^Î (Jora	CICC1=CC(C(O)=O)=CC=
301	130224051501260917042803	3	HJN	NCC1=CC=C(OCO2)C	"	CICC1=CC(C(O)=O)=CC=C1	HAN TOX	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HAI ~ 10	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
302	130224051503260417032807	3		NCC1=CC=C(OCO2)C	"	CICC1=CC(C(O)=O)=CC=C1	H_N~~H_~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	γ	NCC1=CC(OC)=CC(OC)=C1	HO O S	OC([C@H](C)Cl)=O.[S]
303	130224051503260817032802	3	HĮN ()	NCC1=CC=C(OCO2)C	"	CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
304	130224051504260317022809	3	HIN	NCC1=CC=C(OCO2)C	···	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H _L N	NCC1COOCC1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=
305	130224051504260417032810	3	HJN	NCC1=CC=C(OCO2)C	"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H Y ^O	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	NUN COL	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)Cl)=0.[S]
306	130224051509260317102804	3	HIN	NCC1=CC=C(OCO2)C	i <mark>na k</mark> ana kana kana kana kana kana kana k	CICC1=CC(C(O)=O)=CC=C1	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH O	O=C(O)C1=C(C)OC=C1
307	130224051510280217102804	3	HIN	NCC1=CC=C(OCO2)C	"	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	HOLING	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
308	130224061503260817092804	3	H ₂ N	NCC1=CC=CO1	"	CICC1=CC(C(O)=O)=CC=C1	NH ₂	N[C@@H](C)C1=CC=CC=C1	CI C	OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
309	130224071501260217012803	3	NH ₂	NCC1=CC=C(C)C=C1	"	CICC1=CC(C(O)=O)=CC=C1	***	NCC1=CC=C(S(=O)(C)=O)C=C	OH CI	OC(C1=COC(CCI)=N1)=O	нустри	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
310	130224071501260517092804	3	NH ₂	NCC1=CC=C(C)C=C1	"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O	or the second se	OC(C1=CC=C(OCI)C=C1)=0	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
311	130224071501261017032805	3		NCC1=CC=C(C)C=C1	"	CICC1=CC(C(O)=O)=CC=C1	H,M^CC	NCC1=CC=C(CI)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H _L N	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=O.[S]
312	130224071503260417012806	3	NH ₂	NCC1=CC=C(C)C=C1	HO LOTO	CICC1=CC(C(O)=O)=CC=C1	H,N~~H~	NCCNC(C)=0	of the second se	OC(C1=CC=C(CCI)C=C1)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
313	130224091501260417032803	3	н,п	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	H _N N	NCCNC(C)=0	State of the second sec	OC(C1=CC=C(CCI)C=C1)=0	HAI~~V_V	NCCCN1C=CN=C1	S S	OC([C@H](C)Cl)=O.[S]
314	130224091501260517032803	3	ним	NCCCN1C=CN=C1	HO LOTO	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O	o contraction of the second se	OC(C1=CC=C(CCI)C=C1)=0	H,M ~ M ()M	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
315	130224091502260217012809	3	ним	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	" A A A A A A A A A A A A A A A A A A A	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H _k N	NCC1CCOCC1	o= OH	OC(C1=CSC(CCI)=N1)=O
316	130224091502260717032805	3	H,N N N	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	La.m.	NCC1=CC=C(N(C)C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H _A N	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=O.[S]
317	130224091503260317102804	3	н,п	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1	ortice OH	OC(C1=COC(CCI)=N1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
318	130224101501260617022810	3	HN	C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1	OH CI	0C(C1=CC=C(CCI)C=C1)=0	NAL COLOR	NCCC1=CC=C(OC)C(OC)=C1	Ho ¹ Cora	CICC1=CC(C(0)=0)=CC=
319	130224101501260617032802	3	HN	CIONCON	****	CICC1=CC(C(0)=0)=CC=C1	NH ₂	NCC1=CC=CC=C1	of the second se	00(01=00=0(00)(0=01)=0	H ₂ N OH	NCCO	HO CO S	OC([C(gH](C)C)=O.[S]
320	130224101502260717032803	3	HN	CICNCONI	"	CICC1=CC(C(O)=O)=CC=C1	-h Qm	NCC1=CC=C(N(C)C)C=C1	C CH	OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCON1C=CN=C1	HO O S	OC([C@H](C)C)=0.[S]
321	130224101503260217032809	3	HN	C1CNCCN1		CICC1=CC(C(O)=O)=CC=C1	**************************************	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H _k N	NCC1CCOCC1	HO O S	OC([C@H](C)CI)=O.[S]
322	130224101503260717042809	3	HNYNH	C1CNCCN1		CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1	OF OH	OC(C1=CSC(CCI)=N1)=O	H _N N	NCC1CCOCC1	HO CO R	OC([C@H](C)Br)=O.[R]
323	130224101510260317032801	3	HN	CIONCONI	10	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	Hole Contraction	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	NCCC1=CNC2=CC=CC=C21	HO CO S	OC([C@H](C)C)=0.[S]
324	130224101510260317092804	3	HN	C1CNCCN1	****	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	₩ ¹ ¶ [*]	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
325	130324031502260817022810	3	H ₂ N~0	NCCCOC	O= OH	0C(C1=CSC(CG)=N1)=0		N(C@@H)(C)C1=CC=CC=C1	OF OH	0C(C1=CSC(CCI)=N1)=0	RUN CO	NCCC1=CC=C(OC)C(OC)=C1	HO ^Î () ()	CICC1=CC(C(0)=0)=CC=
320	130324031502260617032802	3	H ₂ N	Neccoc				NOBBHIC)C1=CC=CC=C1	O= OH		H ₂ N OH		HO CO S	
327	130324031503260517102804	3	H ₂ N~0	NCCCOC	- Com	OC(C1=CSC(CCI)=N1)=0	H ₂ N OH	NCC(C)(C)O	of the second se	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	↓ ^{OH}	0=C(0)C1=C(C)OC=C1
528	130324031504260517032802	3	H ₂ N~0	NUCCOC	OH OH	00(C1=03C(CCI)=N1)=0		NUC(C)(C)O	of the second se	UU(UT=UU=C(CCI)C=C1)=0	H ₂ N OH	NUCCO	HO O S	ос((ошн)(C)CI)=0.[S]
329	130324031504260817022810	3	11 <u>2</u> N~~_0~	NUCCOC		00(C1=CSC(CCi)=N1)=0	NH ₂	N(U@@H)(C)C1=CC=CC=C1	O= OH	00(C1=CSC(CCI)=N1)=0	HIN CO	NUCC1=CC=C(OC)C(OC)=C1	- ¹ 0^-	UKC1=CC(C(0)=0)=CC=
330	130324041502260217032802	3	MH ₂	NGC=C	OCT OH	00(01=030(001)=N1)=0	MAN Contraction	NUC 1=UC=U(S(=O)(C)=O)C=C	OF OH		H ₂ N OH	NOCOU	HO O S	ооцодиј(с)Cl=0.[S]
331	130324041503260517022809	3	MH ₂	NCC=C	OF OH	00(C1=CSC(CCI)=N1)=0		NUCT=CC=CC=C1	of the second se	UU(CT=UC=C(CCI)C=C1)=0	H ⁱ N-	NGC1000001	HOLOCA	UUU1=CC(C(0)=0)=CC=

332	tull.mol.code2 130324051501260417102804	3		Amines(X1)-smiles NCC1=CC=C(OCO2)C		Acid(X1)-smiles OC(C1=CSC(CCI)=N1)=O		Amines(X2)-smiles		Acid(X2)-smiles OC(C1=CC=C(CCI)C=C1)=O	Amines(X3)	Amines(X3)-smiles N[C@@H](C)C1=CC=CC=C1.[S	OH OH	Pair3.Acids O=C(O)C1=C(C)OC=C1
333	130324051502260617102801	3	H ₂ N	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	o contraction of the second se	OC(C1=CC=C(CCI)C=C1)=O	H,N S	N[C@@H](C)C1=CC=CC=C1.[S		OC(C1=CSC(CCI)=N1)=O
334	130324051503260717032809	3	H _I N CC	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=O.[S]
335	130324051503260817032803	3		NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	O=OH	OC(C1=CSC(CCI)=N1)=O	ни~~~nДо	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
336	130324051503260817102804	3	H _I N CC	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
337	130324051504260517032802	3	H,N CC O	NCC1=CC=C(OCO2)C	o= ()H	OC(C1=CSC(CCI)=N1)=O	H ₂ N H	NCC(C)(C)O	and the second s	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HU U S	CC([C@H](C)Cl)=0.[S]
338	130324051504260617092804	3	H _A N CLO	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
339	130324051509260117032804	3	H _L N C C C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	···	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=O.[S]
340	130324051509260217012803	3	H ₂ N C C C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	HUI C	NOC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H.M.~_N_Dr	NCCCN1C=CN=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O
341	130324051509260217032802	3	H _L N C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NUC C	NCC1=CC=CC(C(F)(F)F)=C1	₩ ¹ ₩	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
342	130324051510260417092804	3	H _A N C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		CC(C)OCN	····	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
343	130324061509260217102804	3	H ₂ N	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O	HUI CON	NCC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
344	130324071501260417032802	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H_N~~H~~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
345	130324071501260817012803	3	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	OH CI	OC(C1=CSC(CCI)=N1)=O	H,H~~Y_	NCCON1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
346	130324071502260317032802	3	NH ₂	NCC1=CC=C(C)C=C1	O=	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	O= OH	OC(C1=COC(OCI)=N1)=O	H ₂ N OH	NCCO	S CI S	OC([C@H](C)CI)=O.[S]
347	130324071503260317092804	3	NH ₂	NCC1=CC=C(C)C=C1	OH OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	O-CI	OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
348	130324071503260817042803	3	NH ₂	NCC1=CC=C(C)C=C1	O=	OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	"" "D"	NCCCN1C=CN=C1	HO O Br R	0C([C@H](C)Br)=0.[R]
349	130324071509260417032801	3	NH ₂	NCC1=CC=C(C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	1.11 J	NCC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN SHE	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)CI)=0.[S]
350	130324071509260417092804	3	NH ₂	NCC1=CC=C(C)C=C1	o= ↓ ∩	OC(C1=CSC(CCI)=N1)=O	1.1 ~ ~ ¹ /	NCC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
351	130324071510260317032804	3	NH ₂	NCC1=CC=C(C)C=C1	OF OH	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1	HO S	CC([C@H](C)Cl)=0.[S]
352	130324081503261017102804	3	HN	N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	H _N	NCC1=CC=C(CI)C=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
353	130324081504260417102804	3	HN	N1CONCCC1	C= CH	OC(C1=CSC(CCI)=N1)=O	H,N~~~ ^H ~0	NCCNC(C)=0		0C(C1=CC=C(CCI)C=C1)=0	HANK S	N[C@@H](C)C1=CC=CC=C1 [S	OH OH	0=C(0)C1=C(C)0C=C1
354	130324081509260417032803	3	HN	N1CONCCC1	OF OH	OC(C1=CSC(CCI)=N1)=O	1.11 ~ ~ ¹ /1	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	"" "D"	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
355	130324081510260417102802	3	HN	N1CONCCC1	OH OH	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	HO ^Î () ^a	CICC1=CC(C(O)=O)=CC=
356	130324091502260317092804	3	H_NN	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	CI CH CH	OC(C1=COC(OCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
357	130324091503260417032802	3	H2N N N	NCOCN1C=CN=C1	OH OH	OC(C1=CSC(CCI)=N1)=O	H _J N N YO	NCCNC(C)=0	of the second se	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	0C([C@H](C)CI)=0.[S]
358	130324091503260717012808	3	H_NN	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1	C CI	OC(C1=CSC(CCI)=N1)=0	H _A N Br	BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCI)=N1)=O
359	130324091503260817022803	3	ни	NCOCN1C=CN=C1	o= OH	OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	CI CI CI	OC(C1=CSC(CCI)=N1)=O	","~~"()"	NCCCN1C=CN=C1	Ho ¹	CICC1=CC(C(0)=0)=CC=
360	130324101502260217102804	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C(S(=0)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	of the second	0=C(0)C1=C(C)0C=C1
361	130324101502260517092804	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H ₂ N H	NCC(C)(C)O	Of the second se	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
362	130324101503260617022803	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	HN~~Y_).	NCCCN1C=CN=C1	"i g~	CICC1=CC(C(0)=0)=CC=
363	130324101504260617022806	3	HN	CTONOCN1	O-CH	OU(C1=CSC(CCI)=N1)=O	NH ₂	NUC1=CC=CC=C1	of the second se	UU(C1=CC=C(CCI)C=C1)=0	NH ₂	NC[C@H](C)C1=OC=OC=C1	Ho ¹	UCC1=CC(C(0)=0)=CC=
364	130324101504260617032802	3	HIN	CTONCON1		UC(C1=CSC(CCI)=N1)=O		NUC1=CC=CC=C1	of the second se	uu(c1=cc=c(ccl)c=c1)=0	H ₂ N OH	NGCO	HO. O S	UC([C@H](C)CI)=0.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair	Pair3.Acids
365	130324101504260617032805	3	HN	C1CNCCN1	o=√H	OC(C1=CSC(OCI)=N1)=O		NCC1=CC=CC=C1	of the second se	0C(C1=CC=C(CCI)C=C1)=0	HIN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=0.[S]
366	130324101509260417042803	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	HUI COL	NCC1=CC=CC(C(F)(F)F)=C1	····	CIC/C(C)=C/[C@@H](C)C(O)=O	HM ~~ 101	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
367	130324101510260317042804	3	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HO TOTAL	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1	HO O Br R	OC([C@H](C)Br)=O.[R]
368	130424021501260617032803	3	H ₂ N	NCC1=CC=CN=C1	₩ ² τ ⁴ γ~a	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	"" "D	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
369	130424021502260817022809	3	H ₂ N	NCC1=CC=CN=C1	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCCCC1	но	CICC1=CC(C(O)=O)=CC=
370	130424021504260717032803	3	H ₂ N N	NCC1=CC=CN=C1	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	-horanne	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HM~~N_N	NCCCN1C=CN=C1	HU U S	OC([C@H](C)Cl)=O.[S]
371	130424031501260117102804	3	H ₂ N	NCCCOC	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N	NCCOC		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	o → → O H O H	O=C(O)C1=C(C)OC=C1
372	130424031501260417092804	3	H ₂ N	NCCCOC	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H_N N	NCCNC(C)=0	OF CI	OC(C1=CC=C(CCI)C=C1)=0	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	∽	CCC(O)=O
373	130424031501261017092804	3	H ₂ N	NCCCOC	HO Land	CIC/C(C)=C/(C@@H)(C)C(O)=O	H _M	NCC1=CC=C(CI)C=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
374	130424031503260217032803	3	H ₂ N	NCCCOC	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAN OF	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	HM NON	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
375	130424031503260617022802	3	H ₂ N	NCCCOC	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	NH ₂	NCC1=CC=CC=C1	o cit	OC(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	но	CICC1=CC(C(O)=O)=CC=
376	130424031503260717032802	3	H ₂ N	NCCCOC	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	-horan and	NCC1=CC=C(N(C)C)C=C1	o=√N OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
377	130424031503261017092803	3	H ₂ N 0	NCCCOC	HO TATA	CIC/C(C)=C/(C@@H)(C)C(O)=O	H,N^CC	NCC1=CC=C(CI)C=C1	HO TO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)CI)=O.[S]
378	130424031504260917102804	3	H ₂ N	NCCCOC	HO TO	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAN TO Y	NOC1=CC(F)=CC(C(F)(F)F)=C		OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
379	130424031509260117042803	3	H ₂ N	NCCCOC	HO TO	CIC/C(C)=C/(C@@H)(C)C(O)=O	HALLOY	NCC1=CC=CC(C(F)(F)F)=C1	HO TATA	CIC/C(C)=C/[C@@H](C)C(O)=O	"" "D'	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
380	130424031509260217032806	3	H ₂ N	NCCCOC	HO TO	CIC/C(C)=C/(C@@H)(C)C(O)=O	with	NCC1=CC=CC(C(F)(F)F)=C1	HO TOTAL	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)CI)=O.[S]
381	130424031510260317102802	3	H ₂ N	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	HO TOTAL	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	HO ^L	CICC1=CC(C(O)=O)=CC=
382	130424041503260417092803	3	NH ₂	NCC=C	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N~~H	NCCNC(C)=O	OF CONTRACTOR	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)CI)=O.[S]
383	130424041504260317102804	3	NH ₂	NCC=C	HO TOTA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1	OF OH	OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
384	130424041504260717102804	3	MH ₂	NCC=C	HO TO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NOC1=CC=C(N(C)C)C=C1	OF OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	↓ ^{OH}	O=C(O)C1=C(C)OC=C1
385	130424051501260617102804	3	HJN	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1=CC=CC	of the second se	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N ₄ s	N[C@@H](C)C1=CC=CC=C1.[S	of the second	0=C(0)C1=C(C)0C=C1
386	130424051502260617022803	3	H,N C C C	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	···~~··D·	NCCCN1C=CN=C1	" ¹ U"	CICC1=CC(C(O)=O)=CC=
387	130424051502260717012806	3	HJN CON	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	A CALINA	NCC1=CC=C(N(C)C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	O=OH	OC(C1=CSC(CCI)=N1)=O
388	130424051503260217032803	3	HIN	NCC1=CC=C(OCO2)C	"	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	ни~~р	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)CI)=0.[S]
389	130424061503261017102803	3	HIN	NCC1=CC=C(0C02)C	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N C	NCC1=CC=C(CI)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)CI)=0.[S]
390	130424051509260117092803	3	HĮN	NCC1=CC=C(OCO2)C	"	CIC/C(C)=C/[C@@H](C)C(0)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	₩ ^Ĺ ŧ ^ĸ Υ	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO CO S	OC([C@H](C)Cl)=O.[S]
391	130424051509260317022809	3	HIN	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	NUT Y	NCC1=CC=CC(C(F)(F)F)=C1	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HOLOCA	CICC1=CC(C(O)=O)=CC=
392	130424061502260317102804	3	H ₂ N O	NCC1=CC=CO1	no la proposi	CiCrC(C)=C/(CB(BH)(C)C(C)=C	H ₂ N S	NCC1=CC=CS1	CH CI	00(01=000(00)=N1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	of the	0=0(0)01=0(0)00=01
393	130424071501260517012803	3	NH ₂	NCC1=CC=C(C)C=C1	10	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N /	NCC(C)(C)O	° ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	ни~~р	NCCCN1C=CN=C1	→ CI	OC(C1=CSC(CCI)=N1)=O
394	130424071501260517032809	3	NH ₂	NUU1=CC=C(C)C=C1		GGG(C)=G/(C@@H)(C)C(O)=O		NUCIC)(C)O	OH CI	UU(G1=UU=C(CCI)C=C1)=0	H ₂ N	NUCTCC0CC1	HO O S	uu([u@H](C)Cl)=0.[S]
395	130424081503260417092804	3	HN	N1CONCCC1	₩ [°] ¥~a	GU/C(C)=G/(C@@H)(C)C(O)=O	H_N ~~- ^H	NUCNC(C)=0		00(C1=CC=C(CCI)C=C1)=0	H ₂ N C n	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CUC(0)=0
390	130424081503260917032808	3	HN	NIGUNCCC1	····	니니니(U)=C/[C(2)(M)(C)C(0)=0	HUNT Y	NUG1=GG(F)=GG(C(F)(F)F)=C	OF OH	UU(UT=USU(CCI)=N1)=0	H _A N Br	BIGT=UG=C(CN)C=C1	HO O S	uu(µgH)(C)CI)=0.(S)
391	190424081504260417032801	3	HIN	NICONCCC1		니다"다(다운(C원@H](C)C(0)=0	н,м~~й~ро	NUCINC(C)=0	OF COLOR	00(01=00=C(CCI)C=C1)=0	H,N	NGCU1=CNC2=CC=CC=C21	HO. O	UU([C@H](C)CI)=0.[S]

398	tull.mol.code2 130424081510260417022805	3		Amines(X1)-smiles N1CCNCCC1		Acid(X1)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O		Amines(X2)-smiles CC(C)CCN		ACid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines(X3)	Amines(X3)-smiles NCC1COC(C=CC=C2)=C2O1	HO CO	Pair3.Acids CICC1=CC(C(O)=O)=CC=
399	130424091501260417102804	3	H_H ~ H_C H	NCCCN1C=CN=C1	10 Proto	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N N YO	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S	o H	0=C(0)C1=C(C)OC=C1
400	130424091501260917102803	3	H ₂ H~~N_N	NCCCN1C=CN=C1	HOLYN	CIC/C(C)=C/[C@@H](C)C(O)=O	HUN TO Y	NOC1=CC(F)=CC(C(F)(F)F)=C1	<u></u>	OC(C1=CSC(CCI)=N1)=O	H _J N	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)Cl)=O.[S]
401	130424091502260217032803	3	""" ~~ """	NCCCN1C=CN=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN COL	NCC1=CC=C(S(=0)(C)=0)C=C	SH CI	OC(C1=COC(CCI)=N1)=O	HW ~~~ W D	NCCCN1C=CN=C1	HO_O_S	OC([C@H](C)Cl)=O.[S]
402	130424091502260317022803	3	H ₂ H~~_HH	NCCCN1C=CN=C1	Holyman	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1	OH Shart	OC(C1=COC(CCI)=N1)=O	H.M.~~10	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=
403	130424091502260517092804	3	нити	NCCCN1C=CN=C1	Holysing	CIC/C(C)=C/(C@@H)(C)C(O)=O		NCC(C)(C)O	°он	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N(C(@H)(C)C1=CC=CC=C1.[R]	\sim	CCC(O)=O
404	130424091502260817032802	3	H ₂ N~~N_N	NCCCN1C=CN=C1	Holy of	CIC/C(C)=C/[C@@H](C)C(O)=O	\mathbf{Q}	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O		NCCO		OC([C@H](C)Cl)=O.[S]
405	130424091504260417032804	3	ни	NCCCN1C=CN=C1	HOLENSTO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N O	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=0.[S]
406	130424091504260517032802	3	H,H~~N_N	NCCCN1C=CN=C1	In ly stra	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O		NCCO		OC([C@H](C)Cl)=0.[S]
407	130424091509260317032805	3	H ₂ N~~N~N	NCCCN1C=CN=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	NA THE	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H _J N	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=O.[S]
408	130424091509260417022810	3	H ₂ N~~N~N	NCCCN1C=CN=C1	1 1	CIC/C(C)=C/[C@@H](C)C(O)=O	wingt	NCC1=CC=CC(C(F)(F)F)=C1	1 I	CIC/C(C)=C/[C@@H](C)C(O)=O	پ اس	NCCC1=CC=C(OC)C(OC)=C1		CICC1=CC(C(O)=O)=CC=
409	130424091510260317032802	3	H ₂ N~~N~N	NCCCN1C=CN=C1	in the second	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	H,N OH	NCCO	HO CO S	OC([C@H](C)Cl)=0.[S]
410	130424091510260417032802	3	020~0~0~N	NCCCN1C=CN=C1	- 1 -	CIC/C(C)=C/[C@@H](C)C(O)=O	L A	CC(C)CCN	n 1 1 1	CIC/C(C)=C/(C@@H)(C)C(O)=O	нихон	NCCO	HO C S	OC([C@H](C)CI)=O.[S]
411	130424101501260817032804	3	HN	C1CNCCN1	lucion a	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N O	NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
412	130424101501261017032809	3		C1CNCCN1	less.	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ NH ₂	NCC1=CC=C(CI)C=C1	о-Кон	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1		OC([C@H](C)Cl)=0.[S]
413	130424101502260217042809	3		C1CNCCN1	i i i	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O		NCC1CCOCC1	HO O R	OC([C@H](C)Br)=O.[R]
414	130424101502260417012806	3		C1CNCCN1	lesin	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=0	o≺ _{oH}	OC(C1=CC=C(CCI)C=C1)=O	\bigcirc	NC[C@H](C)C1=CC=CC=C1	Br Grad	OC(C1=CSC(CCI)=N1)=O
415	130424101503260617012803	3		C1CNCCN1	"IT"	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		NCCCN1C=CN=C1	o≓ oH	OC(C1=CSC(CCI)=N1)=O
416	130424101504260617022808	3		C1CNCCN1	™ ¥¥ ∿	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		BrC1=CC=C(CN)C=C1	o= <on< td=""><td>CICC1=CC(C(O)=O)=CC=</td></on<>	CICC1=CC(C(O)=O)=CC=
417	130424101504260617032805	3		C1CNCCN1	** Y Y Y	CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1COC(C=CC=C2)=C2O1	H0 40 .	OC([C@H](C)Cl)=0.[S]
418	130424101504260817032802	3		C1CNCCN1	™¶¶¶∩ Î.	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CSC(CCI)=N1)=O		NCCO		OC([C@H](C)Cl)=0.[S]
419	130924021502260717032802	3		NCCC1CCOCC1	Real Property of the second se	CICC1=CC(C(O)=O)=CC=C1	J. C	NCC1=CC=C(N(C)C)C=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ²	NCCO	HO_O	OC([C@H](C)Cl)=0.[S]
420	130924021502260717102804	3		NCCC1CCOCC1	i i	CICC1=CC(C(O)=O)=CC=C1	L.	NOC1=CC=C(N(C)C)C=C1	он Сн	OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S		0=C(0)C1=C(C)0C=C1
421	130924021502261017042804	3	H ₂ N	NCCC1CCCCC1	i i	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(CI)C=C1	о-Сон ¥	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1	HO_O	OC([C@H](C)Br)=O.[R]
422	130924021503260417032803	3		NCCC1CCOCC1	HO TOTO	CICC1=CC(C(O)=O)=CC=C1	н	NCCNC(C)=0	**************************************	OC(C1=CC=C(CCI)C=C1)=O		NCCCN1C=CN=C1	HO_O	OC([C@H](C)Cl)=O.[S]
423	130924021504260717092804	3		NECC1CEDEC1	Hotoro P	CICC1=CC(C(0)=0)=CC=C1	H _M N PO	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HAN Y HON	N[C@H](C)C1=CC=CC=C1.[R]		CCC(0)=0
424	130924021504260817102804	3		NCCC1CCOCC1	HO 1000	CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1	он он	OC(C1=CSC(CCI)=N1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S	он	0=C(0)C1=C(C)0C=C1
425	130924021509260417092804	3		NCCC1CCOCC1	8	CICC1=CC(C(O)=O)=CC=C1	J _{NH}	NCC1=CC=CC(C(F)(F)F)=C1	о-Сон	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N-4	N[C@H](C)C1=CC=CC=C1.[R]		CCC(0)=0
426	130924031501260717022802	3		NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	HAN TOX	NCC1=CC=C(N(C)C)C=C1	molyno	OC(C1=CSC(CCI)=N1)=O	۵ «	NCCO	OH	CICC1=CC(C(O)=O)=CC=
427	130924031501260717022804	3	Han	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	10~m	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCC1=CC=CO1	********	CICC1=CC(C(O)=O)=CC=
428	130924031501260817042803	3	H ₂ N	NCCC1CCDCC1	O	OC(C1=CSC(CCI)=N1)=O	^\	N[C@@H](C)C1=CC=CC=C1	O=OH	OC(C1=CSC(CCI)=N1)=0	H ₂ N	NCCCN1C=CN=C1	HO	0C([C@H](C)Br)=0.[R]
429	130924031503260817102804	3	H ₂ N	NCCC1CCOCC1	O= OH	OC(C1=CSC(CCI)=N1)=O	NH,	N[C@@H](C)C1=CC=CC=C1	о= он	OC(C1=CSC(CCI)=N1)=0	H,N	N[C@@H](C)C1=CC=CC=C1.[S	Br	0=C(0)C1=C(C)0C=C1
430	130924031504280317102804	3	H ₂ N	NCCC1CCOCC1	OF OH	OC(C1=CSC(CC1=N1)=0	NH ₂	NCC1=CC=CS1	O-COH	0C(C1=C0C(CCI)=N1)=0	5			0=6(0)61=6(0)60=61
	10002700/1007200317102004		H ₂ N		O= OH	and a constraint lift had.	H ₂ N		OH CI		S s		0 OH	

431	full.mol.code2 130924031504260517032802	3	Amines(X1)	Amines(X1)-smiles NCCC1CCOCC1		Acid(X1)-smiles OC(C1=CSC(CCi)=N1)=O	Amines(02) H ₂ N	Amines(X2)-smiles NOC(C)(C)O		Acid(X2)-smiles OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	Amines(X3)-smites NCCO	HO S	Pair3.Acids OC([C@H](C)Cl)=O.[S]
432	130924031504260817022803	3	Han	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O		N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	w~~_0	NCCCN1C=CN=C1	но ¹ ста	CICC1=CC(C(O)=O)=CC=
433	130924031510260317102802	3	H ₂ N	NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HO ^L T ^S	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	но	CICC1=CC(C(O)=O)=CC=
434	130924041503260317032803	3	H ₂ N	NCCC1CCOCC1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	~~~~v)	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
435	130924041510260117092804	3	H ₂ N	NCCC1CCOCC1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	CCC(O)=O
436	131024011504260717042803	3	HeN	NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCI)=N1)=O	A Carm	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HM~~10	NCCCN1C=CN=C1	HU U R	OC((C@H)(C)Br)=O.[R]
437	131024011510260317102804	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=COC(CCI)=N1)=O		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	o d d d d d d d d d d d d d d d d d d d	O=C(O)C1=C(C)OC=C1
438	131024021501260317102804	3	H ₂ N	NCC1=CC(F)=C(F)C=C		CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH OH	0=C(0)C1=C(C)0C=C1
439	131024021503260417032803	3	H ₂ N	NCC1=CC(F)=C(F)C=C		CICC1=CC(C(O)=O)=CC=C1	H ₂ N N N	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=0	HM~~~D1	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
440	131024031501260617032802	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
441	131024031503260717032802	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	-horana	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
442	131024031503260817012803	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	C NH2	N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	"" "	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
443	131024031504260917022804	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O		NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C01	но	CICC1=CC(C(O)=O)=CC=
444	131024031509260217012803	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	m land	CIC/C(C)=C/[C@@H](C)C(O)=O	ни	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
445	131024031509260317032802	3	Han	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	w	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	S S	OC([C@H](C)CI)=O.[S]
446	131024031510260417102803	3	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	₩ ^L trstra	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)CI)=O.[S]
447	131024041503260417092804	3	H ₂ N	NCC1=CC(F)=C(F)C=C	"	CIC/C(C)=C/[C@@H](C)C(0)=O	H,N~H~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
448	131024041504260817032803	3	Han	NCC1=CC(F)=C(F)C=C		CIC/C(C)=C/[C@@H](C)C(O)=O	NH,	N[C@@H](C)C1=CC=CC=C1	<u>k</u>	OC(C1=CSC(CCI)=N1)=O	HAN	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
449	130124011503260517102804	2	H _L N Br	NCC1=CC=CC(Br)=C1		OC(C1=COC(CCI)=N1)=O		NCC(C)(C)O	CH C	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	of the second	O=C(O)C1=C(C)OC=C1
450	130124011509260317032809	2	H ₂ N Br	NCC1=CC=CC(Br)=C1	C C C C	OC(C1=COC(CCI)=N1)=O	HALL	NCC1=CC=CC(C(F)(F)F)=C1	₩ ¹ ¶*\^a	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=O.[S]
451	130124021502260817022804	2	H ₂ N N	NCC1=CC=CN=C1	OF OH	OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	но	CICC1=CC(C(O)=O)=CC=
452	130124021503260217092804	2	H ₂ N	NCC1=CC=CN=C1		OC(C1=COC(CCI)=N1)=O	w Og	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
453	130124021503261017032801	2	H ₂ N	NCC1=CC=CN=C1		OC(C1=COC(CCI)=N1)=O	HM	NCC1=CC=C(CI)C=C1	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)CI)=O.[S]
454	130124031501260417042809	2	H ₂ N~0	NCCCOC	OF OH	OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H Y ^O	NCCNC(C)=0	€ CH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO CO R	OC([C@H](C)Br)=O.[R]
455	130124031501260717032801	2	H ₂ N~0	NCCCOC	O=OH	OC(C1=COC(CCI)=N1)=O	Å.	NCC1=CC=C(N(C)C)C=C1	S → CI OH	OC(C1=CSC(CCI)=N1)=O		NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=O.[S]
456	130124031501260817022805	2	H ₂ N O	NCCCOC	OF OH	OC(C1=COC(CCI)=N1)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1	orton orton	OC(C1=CSC(CCI)=N1)=O	H _J N	NCC1COC(C=CC=C2)=C2O1	но	CICC1=CC(C(O)=O)=CC=
457	130124031501260817032802	2	H ₂ N~0	NCCCOC	O-CI	OC(C1=COC(CCI)=N1)=O	C NH.	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H _z N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
458	130124031501260817032803	2	H ₂ N~0~	NCCCOC	O=OH	OC(C1=COC(CCI)=N1)=O	Real Provided Action of the second se	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HAI ~ 101	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
459	130124031501261017042803	2	H ₂ N~0	NCCCOC	→ CI → CI → CI	OC(C1=COC(CCI)=N1)=O	HM	NCC1=CC=C(CI)C=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	***~~^{_	NCCCN1C=CN=C1	HO O R	0C([C@H](C)Br)=0.[R]
460	130124031502260217032802	2	H ₂ N~0	NCCCOC		OC(C1=COC(CCI)=N1)=O	HAN DO	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
461	130124031502261017012805	2	112N~~_0~	NCCCOC	O CI	OC(C1=COC(CCI)=N1)=O	HAN	NCC1=CC=C(Cl)C=C1	₩ [°] T ⁺ ~	CIC/C(C)=C/[C@@H](C)C(O)=O	H _N	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
462	130124031503260217032802	2	H ₂ N	NCCCOC	O= OH	OC(C1=COC(CCI)=N1)=O	w	NCC1=CC=C(S(=0)(C)=0)C=C	OF CH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
463	130124031503260217102804	2	H ₂ N~0	NCCCOC		OC(C1=COC(CCI)=N1)=O	**************************************	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	of of	0=C(0)C1=C(C)0C=C1

464	130124031503260417022803	2		NCCCOC		OC(C1=COC(CCI)=N1)=O		Annied/vc/annes		OC(C1=CC=C(CCI)C=C1)=O	HJN NON	Administration Strength Streng		CICC1=CC(C(O)=O)=CC=
465	130124031503260617012803	2	HJN	NCCCOC		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	HAI ~ YOH	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
466	130124031503260717032802	2	H ₂ N O	NCCCOC	O= OH	OC(C1=COC(CCI)=N1)=O	A CALINI	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
467	130124031503260717042803	2	H ₂ N~O	NCCCOC		OC(C1=COC(CCI)=N1)=O	-LO_NH,	NCC1=CC=C(N(C)C)C=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	ни~~~nДо	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
468	130124031504260417022810	2	H ₂ N~O	NCCCOC		OC(C1=COC(CCI)=N1)=O	H _M N	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	N/A	NCCC1=CC=C(OC)C(OC)=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
469	130124031504260817102803	2	H ₂ N	NCCCOC		OC(C1=COC(CCI)=N1)=O	C NH2	N(C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	s s	N[C@@H](C)C1=CC=CC=C1.[S	HU U S	OC([C@H](C)CI)=O.[S]
470	130124031509260217032808	2	H ₂ N O	NCCCOC		OC(C1=COC(CCI)=N1)=O	HUI Y	NCC1=CC=CC(C(F)(F)F)=C1	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N C	BrC1=CC=C(CN)C=C1	HO O S	OC([C@H](C)Cl)=O.[S]
471	130124031509260417012804	2	H ₂ N	NCCCOC	OF OH	OC(C1=COC(CCI)=N1)=O	with	NOC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1	O=OH	OC(C1=CSC(CCI)=N1)=O
472	130124031509260417022805	2	H ₂ N~O	NCCCOC		OC(C1=COC(CCI)=N1)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O	Han	NCC1COC(C=CC=C2)=C2O1	HO ^L	CICC1=CC(C(O)=O)=CC=
473	130124041501260517022804	2	MH ₂	NCC=C	O=OH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1	HO ^L	CICC1=CC(C(O)=O)=CC=
474	130124041501260617032805	2	NH ₂	NCC=C	O= OH	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1	°↓↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=O.[S]
475	130124041501260817032807	2	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O		N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	₹ ↓	NCC1=CC(OC)=CC(OC)=C1	HO S	ос([C@H](C)CI)=O.[S]
476	130124041501260917022809	2	NH ₂	NCC=C	O O OH	OC(C1=COC(CCI)=N1)=O	"	NOC1=CC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HOLOCO	CICC1=CC(C(O)=O)=CC=
477	130124041502260417042805	2	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H,N~H~	NCCNC(C)=0	°↓↓↓ ⊂	OC(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCC1COC(C=CC=C2)=C2O1	HO O Br R	OC([C@H](C)Br)=O.[R]
478	130124041502260517022803	2	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N VH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=0	"" "	NCCCN1C=CN=C1	HO ^Î ()	CICC1=CC(C(O)=O)=CC=
479	130124041502260617032802	2	MH ₂	NCC=C	OF OH	OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	°↓↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
480	130124041502260917032802	2	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	with the second se	NOC1=CC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=0.[S]
481	130124041503260317032802	2	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
482	130124041503260617032801	2	NH ₂	NCC=C	O= OH	OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	°↓↓↓↓↓	0C(C1=CC=C(CCI)C=C1)=0	ни	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)CI)=O.[S]
484	130124041503260717032806	2	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1	OF CH	OC(C1=CSC(CCI)=N1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)Cl)=O.[S]
485	130124041503260817092804	2	MH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	СНОН	CCC(O)=O
486	130124041503260917032802	2	NII2	NCC=C	O= OH	OC(C1=COC(CCI)=N1)=O	HUIT OF Y	NOC1=CC(F)=OC(C(F)(F)F)=C1	o≓ OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ^{OH}	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
487	130124041504260417022805	2	NH ₂	NCC=C		OC(C1=COC(CCI)=N1)=O	H _N N	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N Y	NCC1COC(C=CC=C2)=C2O1	HO	CICC1=CC(C(O)=O)=CC=
488	130124051501260717032802	2	H _k N CC 0	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	A CALINA	NCC1=CC=C(N(C)C)C=C1	o≓ OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
489	130124051501260917032810	2	H,N CC O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	HUN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1	o=√oH	OC(C1=CSC(CCI)=N1)=O	N/ C	NCCC1=CC=C(OC)C(OC)=C1	HO O S	0C([C@H](C)CI)=0.[S]
490	130124051501261017032809	2	H,N CCC	NCC1=CC=C(0C02)C		OC(C1=COC(CCI)=N1)=O	HAN	NCC1=CC=C(CI)C=C1	HO ^L TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N0C1CC0CC1	HO O S	0C([C@H](C)CI)=0.[S]
491	130124051502260217102802	2	H _k N CC 0	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=0	"	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	HAN S	N[C@@H](C)C1=CC=CC=C1.[S	Hold Contraction	CICC1=CC(C(0)=0)=CC=
492	130124051502260317032806	2	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=0	H ₂ N S	NCC1=CC=CS1	o=↓ OH	OC(C1=COC(CCI)=N1)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO S	oc([C@H](C)Cl)=0.[S]
493	130124051502260317042804	2	H _A N	NCC1=CC=C(OCO2)C	→ → ∩ CI	OC(C1=COC(CCI)=N1)=O	H ₂ N S	NOC1=CC=CS1	→ → CI → → → CI	OC(C1=COC(CCI)=N1)=O	H ₂ N C	NCC1=CC=CO1	HO O Br R	0C([C@H](C)Br)=0.[R]
494	130124051502260517032802	2	H,N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N H	NCC(C)(C)0	CH CI	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO C S	0C([C@H](C)Cl)=0.[S]
495	130124051502260617032802	2	H,N CCO	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N ~- OH	NCCO	HO S	0C([C@H](C)Cl)=0.[S]
496	130124051502260717102802	2	H _k N C C O	NCC1=CC=C(OCO2)C		UU(C1=COC(CCI)=N1)=O		NUC1=CC=C(N(C)C)C=C1	O= OH	00(C1=CSC(CCI)=N1)=0	H ₂ N S	NUCEOHIC)C1=CC=CC=C1.[S	HO LOCA	GICC1=CC(C(0)=0)=CC=
497	130124051502261017092804	2	H _N , CLO	INCC1=CC=C(OCO2)C		UU(CT=CUC(CCI)=N1)=0	H ⁱ N, JO ⁰	NUCT=CC=C(CI)C=C1	₩ ^Î ţ ^s tra	uuru(u)=u{C@@H](C)C(O)=O	H ₂ N R	м[U@H](C)C1=CC=CC=C1.[R]	OH	00000

498	130124051503260317102804	2	H _N N CCC	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H _J N	N[C@@H](C)C1=CC=CC=C1.[S	otho otho	0=C(0)C1=C(C)0C=C1
499	130124051503260417022809	2	H,N C C C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H _k N N YO	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	ноц	CICC1=CC(C(O)=O)=CC=
500	130124051504260417042809	2	H _I N C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	H _N ~ ^H Y ⁰	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO O R	OC([C@H](C)Br)=O.[R]
501	130124051504260817032802	2		NCC1=CC=C(OCO2)C		0C(C1=C0C(CCI)=N1)=0		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
502	130124051504260917022803	2	HAN	NCC1=CC=C(OCO2)C		0C(C1=C0C(CCI)=N1)=0	HAR OF T	NOC1=CC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HAN YON	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
503	130124051509260117042801	2	H,N C C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	HAR CON	NOC1=CC=CC(C(F)(F)F)=C1	m from	CIC/C(C)=C/[C@@H](C)C(O)=O	H _M	NCCC1=CNC2=CC=CC=C21	HU R Br	OC([C@H](C)Br)=O.[R]
504	130124051509260217022808	2	H,N C	NCC1=CC=C(OCO2)C		0C(C1=C0C(CCI)=N1)=O	nu t	NOC1=CC=CC(C(F)(F)F)=C1	m to the second	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N ^A CA _{Br}	BrC1=CC=C(CN)C=C1	но	CICC1=CC(C(O)=O)=CC=
505	130124051509260217032802	2	H,N C C C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	nut the	NCC1=CC=CC(C(F)(F)F)=C1	·····	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
506	130124061509260317012801	2	H,N C C	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO I	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21		OC(C1=CSC(CCI)=N1)=O
507	130124051509260417012804	2	H,N C C C	NCC1=CC=C(OCO2)C.		OC(C1=COC(CCI)=N1)=O	nut the	NCC1=CC=CC(C(F)(F)F)=C1	·····	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
508	130124051510260117012803	2	H _N C	NCC1=CC=C(OCO2)C.		OC(C1=COC(CCI)=N1)=O		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	HM ~ 101	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
509	130124051510260117102804	2	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	₩ ^l tsta	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	of the second se	O=C(O)C1=C(C)OC=C1
511	130124061502260317022803	2	HyN	NCC1=CC=CO1	o= oH	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CS1	o= ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=COC(CCI)=N1)=O	····~~	NCCCN1C=CN=C1	носто	CICC1=CC(C(O)=O)=CC=
512	130124061502260617022803	2	H ₂ N	NCC1=CC=CO1		DC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	° ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	HAI YO	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
513	130124061502260717102803	2	H ₂ N O	NCC1=CC=CO1		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S	S	OC([C@H](C)Cl)=O.[S]
514	130124061504260417092804	2	H ₂ N	NCC1=CC=CO1		DC(C1=COC(CCI)=N1)=O	H _N N	NCCNC(C)=0	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
515	130124061509260317022803	2	H ₂ N	NCC1=CC=CO1		OC(C1=COC(CCI)=N1)=O	nu t	NCC1=CC=CC(C(F)(F)F)=C1	Hole Contraction	CIC/C(C)=C/[C@@H](C)C(O)=O	1.vi~10.	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
516	130124071501260217032805	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	"	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	HAN	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=0.[S]
517	130124071501260317012810	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HUN COL	NCCC1=CC=C(OC)C(OC)=C1		OC(C1=CSC(CCI)=N1)=O
518	130124071501260317092803	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	orton CI Orton	OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)Cl)=O.[S]
519	130124071501260417032802	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N~ ^H	NCCNC(C)=O	° ↓ ↓ ↓ ↓ ↓ ↓	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
520	130124071501260517102802	2	NH,	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N ^{OH}	NCC(C)(C)O	- Contraction	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	но ¹ СС-сі	CICC1=CC(C(O)=O)=CC=
521	130124071501260717022807	2	NH ₂	NCC1=CC=C(C)C=C1		DC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	· ↓ · · ·	NCC1=CC(OC)=CC(OC)=C1	но	CICC1=CC(C(O)=O)=CC=
522	130124071501260717042804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO R	OC([C@H](C)Br)=O.[R]
523	130124071501260817022803	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HAN YON	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
524	130124071501260817032802	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	ос([C@H](C)Cl)=0.[S]
525	130124071501261017012801	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	HĨN CI	NOC1=CC=C(CI)C=C1	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ H	NOCC1=CNC2=CC=CC=C21		OC(C1=CSC(CCI)=N1)=O
526	130124071501261017092804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N ¹ Cl	NCC1=CC=C(CI)C=C1	Holy of	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
527	130124071502260317032801	2	NH ₂	NCC1=CC=C(C)C=C1		DC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H _A N Jun	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)Cl)=O.[S]
528	130124071502260417022805	2	NH ₂	NCC1=CC=C(C)C=C1		0C(C1=C0C(CCI)=N1)=0	H ₂ N~ ^H / ^O	NCCNC(C)=0	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ⁴ C	NCC1COC(C=CC=C2)=C2O1	ностори	CICC1=CC(C(O)=O)=CC=
529	130124071502260517042803	2	NH ₂	NCC1=CC=C(C)C=C1		0C(C1=C0C(CCI)=N1)=0	H ₂ N /	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	HAI~~YY	NCCCN1C=CN=C1	HO O R	0C([C@H](C)Br)=0.[R]
530	130124071502260617032806	2	NH ₂	NCC1=CC=C(C)C=C1		DC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	°↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[0@H](C)C1=CC=CC=C1	HO S	OC([C@H](C)CI)=O.[S]
531	130124071502260817022802	2		NCC1=CC=C(C)C=C1		DC(C1=COC(CCI)=N1)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	ноците	CICC1=CC(C(O)=O)=CC=

532	130124071502261017032805	2	Amines(X1)	Amines(X1)-smiles NCC1=CC=C(C)C=C1		Acid(X1)-smiles OC(C1=COC(CCI)=N1)=O	Amines(X2)	Amines(X2)-smiles NOC1=CC=C(CI)C=C1	Acid(X2)	Acid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O		Amines(X3)-smiles NCC1COC(C=CC=C2)=C2O1		Pair3.Acids OC([C@H](C)Cl)=O.[S]
533	130124071503260317022808	2		NCC1=CC=C/C)C=C1	o≓ OH	00(01=000(001)=N1)=0		NCC1=CC=CS1		00(01=000(001)=N1)=0	Ŭ	Brc1=CC=C/CNVC=C1	<u></u>	00001=000000=00=00=
		-		1001-00-0(0)0-01	o= OH		H ₂ N		o= OH		H ₂ N		HO CONTRACTOR	
534	130124071503260517032802	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	°↓↓↓↓↓	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO O S	0C([C@H](C)CI)=0.[S]
535	130124071503260717092804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	-Long	NOC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H,N	N[C@H](C)C1=CC=CC=C1.[R]	OH	CCC(O)=O
536	130124071503260817032802	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
537	130124071503260817032804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N O	NCC1=CC=CO1	HU U S	OC([C@H](C)Cl)=0.[S]
538	130124071503260917012805	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HUN	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
539	130124071503260917102804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O	NA CAL	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N ₄ s	N(C@@H)(C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
540	130124071504260317032802	2	NH ₂	NCC1=CC=C(C)C=C1	`он	OC(C1=COC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
541	130124071504260817032802	2	NH ₂	NCC1=CC=C(C)C=C1	OH J	OC(C1=COC(CCI)=N1)=O	Q	N[C@@H](C)C1=CC=CC=C1	SH CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
542	130124071504260817032807	2		NCC1=CC=C(C)C=C1	OH Shar	OC(C1=COC(CCI)=N1)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	~~~~ ^{\\\}	NCC1=CC(OC)=CC(OC)=C1	HO O S	OC([C@H](C)Cl)=0.[S]
543	130124071509260117012803	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=0	NH ₂	NCC1=CC=CC(C(F)(F)F)=C1	стон ноците	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCON1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
544	130124071509260117012807	2		NCC1=CC=C(C)C=C1	ото Сн Срасси	OC(C1=COC(CCI)=N1)=O	HAR Y Y	NOC1=CC=CC(C(F)(F)F)=C1	"lynyna	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~ [™]	NCC1=CC(OC)=CC(OC)=C1	о= он ул сі	OC(C1=CSC(CCI)=N1)=O
545	130124071509260117032807	2		NCC1=CC=C(C)C=C1	OH SH	OC(C1=COC(CCI)=N1)=O		NOC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1		OC([C@H](C)Cl)=0.[S]
546	130124071509260217032802	2		NCC1=CC=C(C)C=C1	остон уруга	OC(C1=COC(CCI)=N1)=O	www.x	NOC1=CC=CC(C(F)(F)F)=C1	1 I	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N OH	NCCO		OC([C@H](C)Cl)=O.[S]
547	130124071509260317022807	2		NCC1=CC=C(C)C=C1	o≓(oH	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	- 1 ·	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~~~ ^{N4}	NCC1=CC(OC)=CC(OC)=C1		CICC1=CC(C(O)=O)=CC=
548	130124071509260317032802	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=0		NCC1=CC=CC(C(F)(F)F)=C1	lucia	CIC/C(C)=C/[C@@H](C)C(O)=O	K CH	NCCO	HO_FO	OC([C@H](C)Cl)=0.[S]
549	130124071509260317032809	2		NCC1=CC=C(C)C=C1	o≓(oH	OC(C1=COC(CCI)=N1)=O	- U ,	NCC1=CC=CC(C(F)(F)F)=C1	** * * *	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1	HO_O	OC([C@H](C)Cl)=0.[S]
550	130124071510260117032801	2		NCC1=CC=C(C)C=C1	o= on on	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	**************************************	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21	HO_O	OC([C@H](C)CI)=0.[S]
551	130124071510260217032809	2		NCC1=CC=C(C)C=C1	о- он	OC(C1=COC(CCI)=N1)=0		CC(C)CCN	**************************************	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1CCOCC1	ноо	OC([C@H](C)Cl)=0.[S]
552	130124071510260317032803	2		NCC1=CC=C(C)C=C1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCCN1C=CN=C1	HO_O	OC([C@H](C)Cl)=0.[S]
553	130124081501260417042803	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=O		NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	101 - Ch	NCCCN1C=CN=C1	HO. 20	OC([C@H](C)Br)=O.[R]
554	130124081501260517022809	2		N1CONCCC1	O=OH	OC(C1=COC(CCI)=N1)=0	H/W-~~ ^H /~	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=0	······································	NCC1CCOCC1	Br R	CICC1=CC(C(0)=0)=CC=
555	130124081501260617012803	2	HN	N1CONCCC1		0C(C1=C0C(CC1)=N1)=0	H ₂ N /	NCC1=CC=CC=C1	of the second	00(01=00=0(00))0=01)=0	H _k N	NCCCN1C=CN=C1	******	OC/C1=CSC/CCI)=N1)=O
556	130124081502260117012804	2	HN	NICONCOCI	OH OH	0C(C1=C0C(CC1)=N11=0	NH ₂	NCCOC		00(01=000(001)=N(1)=0	HW	NCC1=CC=CO1	OF OH	0C/C1=CSC/CC1=N11=0
			HIN		O=OH		H ₂ N				H ₂ N		O=OH	
55/	130124081502260217032802	2	HN	NICONCOCI	or OH	00(01=000(00)=N1)=0	" Contraction of the second se	NOC1=CC=C(S(=U)(C)=U)C=C		00(C1=C0C(CC)=N1)=0	H ₂ N OH	NGCU	HO S	CC[C@H](C)C)=O.[S]
558	130124081502260417102804	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=0	H ₂ N N Y O	NCCNC(C)=0	OH CI	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[8	OH OH	0=C(0)C1=C(C)0C=C1
559	130124081502260617032806	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	NH ₂	NOC1=CC=CC=C1	ON CI	OC(C1=CC=C(CCI)C=C1)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO S	CC([C@H](C)Cl)=0.[S]
560	130124081502260817022802	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	но	CICC1=CC(C(O)=O)=CC=
561	130124081502260917042804	2	HN	N1CONCCC1		OC(C1=COC(CCI)=N1)=O	HAR THE	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO O Br R	OC([C@H](C)Br)=O.[R]
562	130124081503260417032805	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	n_n~~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	HAN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=0.[S]
563	130124081503260617102804	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
564	130124081503260717012803	2		N1CONCCC1		OC(C1=COC(CCI)=N1)=O	1. June	NCC1=CC=C(N(C)C)C=C1	J. Contraction	OC(C1=CSC(CCI)=N1)=O	~ ++/~~~_	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
					OH				OH				OH	

565	tuil.moi.code2 130124081503260717022803	2		Amines(X1)-smiles N1CCNCCC1	Acid(X1)-smiles OC(C1=COC(CCI)=N1)=0	Amines(X2)	Amines(X2)-smiles NCC1=CC=C(N(C)C)C=C1		Acid(X2)-smiles OC(C1=CSC(CCI)=N1)=0		Amines(X3)-smiles NCCCN1C=CN=C1	HO ¹ CI	Pairs.Acids CICC1=CC(C(O)=O)=CC=
566	130124081503260717032805	2	HN	N1CCNCCC1	OC(C1=COC(CCI)=N1)=O	A COLINHI	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	Han	NCC1COC(C=CC=C2)=C2O1	s of the second	OC([C@H](C)Cl)=O.[S]
567	130124081503260817022809	2	HN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO ^L	CICC1=CC(C(O)=O)=CC=
568	130124081504260117032801	2		N1CONCCC1	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCCOC	o= OH	OC(C1=COC(CCI)=N1)=O	H,H	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)CI)=O.[S]
569	130124081504260217032802	2	HIN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O	HAN CON	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
570	130124081504260217092804	2		N1CONCCC1	OC(C1=COC(CCI)=N1)=O	HAN Of	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(OCI)=N1)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]	~Он	CCC(O)=O
571	130124081504260417012807	2	HIN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O	ни~Нто	NOCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1		OC(C1=CSC(CCI)=N1)=O
572	130124081504260417032801	2		N1CCNCCC1	OC(C1=COC(CCI)=N1)=O	H,N~~H~o	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=0	ни	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)CI)=O.[S]
573	130124081504260517032802	2		N1CCNCCC1	OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
574	130124081504260517092804	2	HIN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	~ рон	CCC(O)=O
575	130124081504260817032806	2		N1CONCCC1	OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO S	OC([C@H](C)CI)=O.[S]
576	130124081509260217102803	2	HN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N(C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)CI)=O.[S]
577	130124081509260317012808	2	HN	N1CCNCCC1	OC(C1=COC(CCI)=N1)=O	HAR TOX	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N Br	BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCI)=N1)=O
578	130124081510260117012809	2	HN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HOLINA	CIC/C(C)=C/[C@@H](C)C(O)=O	HJN	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
579	130124081510260317032808	2		N1CCNCCC1	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N Br	BrC1=CC=C(CN)C=C1	S S	OC([C@H](C)CI)=O.[S]
580	130124081510260317102801	2	HN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N(C@@H](C)C1=CC=CC=C1.[S		OC(C1=CSC(CCI)=N1)=O
581	130124081510260317102803	2	HN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO TO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)CI)=O.[S]
582	130124081510260417012805	2	HIN	N1CONCCC1	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	HyN	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
583	130124091501260417032807	2	H ₂ H~~N_N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H,N~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	γ	NCC1=CC(OC)=CC(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]
584	130124091501260817022810	2	ни	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	NH ₂	N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	нуг-~ССС <mark>.</mark> .	NCCC1=CC=C(OC)C(OC)=C1	HO ^L COCO	CICC1=CC(C(O)=O)=CC=
585	130124091501260917092804	2	H ¹ H	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	NN YY	NOC1=CC(F)=CC(C(F)(F)F)=C1	O=OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
586	130124091502260217022809	2	H ^N N NCM	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	"	NCC1=CC=C(S(=0)(C)=0)C=C	Q Q OH	OC(C1=COC(CCI)=N1)=O	HJN	NCC1CCOCC1	но ⁻¹ -СС о	CICC1=CC(C(O)=O)=CC=
587	130124091502260317022806	2	H ¹ H	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	OF CI	OC(C1=COC(CCI)=N1)=O	NH ₂	NC[C@H](C)C1=CC=OC=C1	но	CICC1=CC(C(O)=O)=CC=
588	130124091502260317032803	2	H2H N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	O-CI OH	OC(C1=COC(CCI)=N1)=O	H.VI~~100	NCCCN1C=CN=C1	HO CO S	OC([C@H](C)Cl)=0.[S]
589	130124091502260417042809	2	H2H N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H _A N~ ^H ¢ ⁰	NCCNC(C)=O	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO O R	OC([C@H](C)Br)=O.[R]
590	130124091502260517032803	2	H2N N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H.N.~~N_)V	NCCCN1C=CN=C1	HO O S	ос([C@H](C)CI)=0.[S]
591	130124091502260717032810	2	H2H~~~HH	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1	CI C	OC(C1=CSC(CCI)=N1)=O	RUN CO	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)CI)=O.[S]
592	130124091502260817042806	2	н,п~~п~п	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	NH ₂	NC[C@H](C)C1=CC=OC=C1	HO O R	OC([C@H](C)Br)=O.[R]
593	130124091503260617032802	2	H ₂ N N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
594	130124091504260417032810	2	H ₂ N N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H,N~~~ ^H ~°	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	HAN CO	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
595	130124091504260517032804	2	н,м	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O		0C(C1=CC=C(CCI)C=C1)=0	H ₃ N	NCC1=CC=CO1	HO O S	ОС([C@H](C)Cl)=0.[S]
596	130124091504260517032808	2	нистр	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O		0C(C1=CC=C(CCI)C=C1)=0	H _A N Constraints	BrC1=CC=C(CN)C=C1	HO S	OC([C@H](C)Cl)=O.[S]
597	130124091509260417012805	2	H2N N	NCCCN1C=CN=C1	OC(C1=COC(CCI)=N1)=O	NN C	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O

598	130124091510260117022809	2		NCCCN1C=CN=C1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO LANG	ACID(XC)-3111165 CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1		CICC1=CC(C(O)=O)=CC=
599	130124101501260117032801	2	HN	C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCCOC		CC(C1=COC(CCI)=N1)=O	B	NCCC1=CNC2=CC=CC=C21	HO S	0C([C@H](C)Cl)=0.[S]
600	130124101501260217032802	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=O)(C)=O)C=C	OH J N	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HOOS	OC([C@H](C)Cl)=O.[S]
601	130124101501260217032804	2		C1CNCCN1	OH	OC(C1=COC(CGI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=0)(C)=0)C=C	он С	OC(C1=COC(CCI)=N1)=O	H ₂ N C	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=0.[S]
602	130124101501260317102804	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	oH of the	O=C(O)C1=C(C)OC=C1
603	130124101501260617032801	2		C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	° €H	OC(C1=CC=C(CCI)C=C1)=O	8	NCCC1=CNC2=CC=CC=C21	HUUUS	OC([C@H](C)Cl)=0.[S]
604	130124101501260617042807	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		NCC1=CC(OC)=CC(OC)=C1	HO C R	OC([C@H](C)Br)=O.[R]
605	130124101501261017032809	2		C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O	H _M	NCC1=CC=C(Cl)C=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	HJN CO	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=0.[S]
606	130124101502260217022805	2		C1CNCCN1	с он	OC(C1=COC(CCI)=N1)=O	why	NCC1=CC=C(S(=0)(C)=0)C=C	J. C	OC(C1=COC(CCI)=N1)=O	H _A N	NCC1COC(C=CC=C2)=C2O1	·····	CICC1=CC(C(0)=0)=CC=
607	130124101502260217092803	2		C1CNCCN1	OH CH	OC(C1=COC(CCI)=N1)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)CI)=0.[S]
608	130124101502260617092803	2		C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	т он	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)CI)=0.[S]
609	130124101502260817032805	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	\mathbf{Q}	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=0	H,N Y	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=0.[S]
610	130124101503260417012804	2		C1CNCCN1	тон С	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCCNC(C)=0	тон С	OC(C1=CC=C(CCI)C=C1)=O		NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
611	130124101503260717042803	2		C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O	40.00	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HALL	NCCCN1C=CN=C1	HO R	OC([C@H](C)Br)=O.[R]
612	130124101503260917032803	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	HUNTON'	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=0	1.01~~1 ₀ 1	NCCCN1C=CN=C1		OC([C@H](C)CI)=O.[S]
613	130124101503260917032804	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	1 1000	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=0.[S]
614	130124101504260317012809	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
615	130124101504260517032802	2		C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	• OH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
616	130124101504260617032802	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
617	130124101504260917032803	2	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	HAN THE	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HAI ~ 101	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
618	130124101504261017032805	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	H,N C	NCC1=CC=C(CI)C=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	H _N N	NCC1COC(C=CC=C2)=C2O1	HOOS	OC([C@H](C)Cl)=O.[S]
619	130124101509260317012804	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	wr DY	NCC1=CC=CC(C(F)(F)F)=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N 0	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
620	130124101509260417012809	2		C1CNCCN1		OC(C1=COC(CCI)=N1)=O	1.11 × 1	NOC1=CC=CC(C(F)(F)F)=C1	HO ^L T ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H _J N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
621	130124101509260417032809	2	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O	NUMAY	NCC1=CC=CC(C(F)(F)F)=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	HIN	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=O.[S]
622	130124101510260317012809	2	HN	C1CNCCN1		OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HO ^L TATO	CIC/C(C)=C/[C@@H](C)C(O)=O	H _k N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
623	130124101510260317092802	2		C1CNCCN1	OH	OC(C1=COC(CCI)=N1)=O		CC(C)CCN	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	юн	CICC1=CC(C(O)=O)=CC=
624	130224011502260617032810	2	H ₂ N Br	NCC1=CC=CC(Br)=C1	юн но ^с сто	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0		NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)Cl)=O.[S]
625	130224011502260717032803	2	H _L N Br	NCC1=CC=CC(Br)=C1	100 m	CICC1=CC(C(O)=O)=CC=C1	1. (), m,	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HAI ~ 10	NCCCN1C=CN=C1	HOOS	OC([C@H](C)Cl)=O.[S]
626	130224011504260817022803	2	H ₂ N Br	NCC1=CC=CC(Br)=C1		CICC1=CC(C(O)=O)=CC=C1	9	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	***~~Y	NCCCN1C=CN=C1	Ho ¹ () ()	CICC1=CC(C(O)=O)=CC=
627	130224021501260417092803	2	H ₂ N N	NCC1=CC=CN=C1	No Contra	CICC1=CC(C(O)=O)=CC=C1		NCCNC(C)=0	OH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HOOS	OC([C@H](C)Cl)=O.[S]
628	130224021501260717012803	2	H ₂ N N	NCC1=CC=CN=C1	-1 ₀ -0	CICC1=CC(C(O)=O)=CC=C1	ham	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
629	130224021502260417102804	2	H ₂ N N	NCC1=CC=CN=C1		CICC1=CC(C(O)=O)=CC=C1	H _N N	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N(C@@H)(C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
630	130224021502260517092804	2	H ₂ N	NCC1=CC=CN=C1		CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC(C)(C)O	• ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	С	CCC(0)=0

631	130224021503260217032802	2	H ₂ N	Amines(X1)-smiles NCC1=CC=CN=C1		Acid(X1)-smiles CICC1=CC(C(O)=O)=CC=C1	Amines(X2)	Amines(A2)-smiles NCC1=CC=C(S(=0)(C)=O)C=C		Add(X2)-smiles OC(C1=COC(CCI)=N1)=O	H ₂ N OH	Amines(X3)-smites	HO S	Pair3.Acids OC([C@H](C)Cl)=O.[S]
632	130224021510260117102804	2	H ₂ N	NCC1=CC=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	······································	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S	ot ot	0=C(0)C1=C(C)OC=C1
633	130224031501260317022803	2	H ₂ N	NCCCOC	10	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HAN	NCCCN1C=CN=C1	HO ¹	CICC1=CC(C(O)=O)=CC=
634	130224031501260317032804	2	H ₂ N	NCCCOC		CICC1=CC(C(O)=O)=CC=C1	H ₂ N S	NCC1=CC=CS1	o= OH	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)CI)=O.[S]
635	130224031501260417032802	2	H ₂ N O	NCCCOC	"	CICC1=CC(C(O)=O)=CC=C1	H _M ^H	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
636	130224031501260617012805	2	H ₂ N~0~	NCCCOC		CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		NCC1COC(C=CC=C2)=C2O1	o= OH	OC(C1=CSC(CCI)=N1)=O
637	130224031501260717032802	2	H ₂ N O	NCCCOC	HO CON	CICC1=CC(C(O)=O)=CC=C1	Å.	NCC1=CC=C(N(C)C)C=C1	O=OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
638	130224031501261017022810	2	H ₂ N O	NCCCOC	***	CICC1=CC(C(O)=O)=CC=C1	H,N^C	NCC1=CC=C(CI)C=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	nur Che	NCCC1=CC=C(OC)C(OC)=C1	HO ¹	CICC1=CC(C(O)=O)=CC=
639	130224031502260717032802	2	H ₂ N~0~	NCCCOC	"	CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1	O=OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
640	130224031503260717032801	2	H ₂ N O	NCCCOC	10 10 10 10 10 10 10 10 10 10 10 10 10 1	CICC1=CC(C(O)=O)=CC=C1	Å.	NCC1=CC=C(N(C)C)C=C1	S CI CH CH	OC(C1=CSC(CCI)=N1)=O	нл	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=O.[S]
641	130224031503260817042803	2	H ₂ N~0~	NCCCOC	*******	CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1	Q= OH CI	OC(C1=CSC(CCI)=N1)=O	ни Мо	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
642	130224031504260317032802	2	H ₂ N O	NCCCOC	···	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1	o=↓ OH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	0C([C@H](C)Cl)=0.[S]
643	130224031504260417022810	2	H ₂ N~~~_0~~	NCCCOC	*********	CICC1=CC(C(O)=O)=CC=C1	H _M N~ ^H ^H	NCCNC(C)=O	° ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=0	N/M COL	NCCC1=CC=C(OC)C(OC)=C1	HO ¹ OCO	CICC1=CC(C(O)=O)=CC=
644	130224031509260217102801	2	H ₂ N O	NCCCOC	"	CICC1=CC(C(O)=O)=CC=C1	NA CAR	NOC1=CC=CC(C(F)(F)F)=C1	···	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N(C@@H)(C)C1=CC=CC=C1.[S	O-CI	OC(C1=CSC(OCI)=N1)=O
645	130224031509260317032805	2	H ₂ N	NCCCOC	"	CICC1=CC(C(O)=O)=CC=C1	NA CA	NCC1=CC=CC(C(F)(F)F)=C1	····	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1	S	OC([C@H](C)Cl)=O.[S]
646	130224031509260417092803	2	H ₂ N	NCCCOC	HO CO	CICC1=CC(C(O)=O)=CC=C1	w	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)Cl)=O.[S]
647	130224041501260417012809	2	NH ₂	NCC=C	"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H ^O	NCCNC(C)=O	° ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	HaN	NCC1CCOCC1	O= OH	OC(C1=CSC(CCI)=N1)=O
648	130224041502260217032802	2	MH ₂	NCC=C	"	CICC1=CC(C(O)=O)=CC=C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=0)(C)=0)C=C	CI CH CH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
649	130224041502260317032804	2	NH ₂	NCC=C	10	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1	of o	OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=O.[S]
650	130224041502260417022803	2	MH ₂	NCC=C		CICC1=CC(C(O)=O)=CC=C1	H ₂ N ^H ^O	NCCNC(C)=O	• ↓ ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	H.M.~~N_)N	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=
651	130224041502260617012809	2	NH ₂	NCC=C	""	CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O
652	130224041502260717032805	2	NII ₂	NCC=C	" ⁱ "	CICC1=CC(C(O)=O)=CC=C1	-horm	NCC1=CC=C(N(C)C)C=C1	ortor of the second se	OC(C1=CSC(CCI)=N1)=O	HANNAR	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=0.[S]
653	130224041503260217102803	2	NH ₂	NCC=C	HO CON	CICC1=CC(C(O)=O)=CC=C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=O)(C)=O)C=C	O-OH	OC(C1=COC(CCI)=N1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	HO O S	OC([C@H](C)Cl)=O.[S]
654	130224041503260317102804	2	NH ₂	NCC=C		CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	ot oth	O=C(O)C1=C(C)OC=C1
655	130224041503261017032803	2	MH ₂	NCC=C	10	CICC1=CC(C(O)=O)=CC=C1	H _A N CO	NCC1=CC=C(CI)C=C1	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN YON	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
656	130224041504260517032802	2	NH ₂	NCC=C	**************************************	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
657	130224041509260317022807	2	NH ₂	NCC=C	10	CICC1=CC(C(O)=O)=CC=C1	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	$\operatorname{Are}_{\mathcal{A}}$	NCC1=CC(OC)=CC(OC)=C1	HO ^Î () ()	CICC1=CC(C(O)=O)=CC=
658	130224041509260417022803	2	NH ₂	NCC=C	""	CICC1=CC(C(O)=O)=CC=C1	HALL CAL	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CiCrC(C)=Cr[C@@H](C)C(O)=O	H,H ~ Y Y	NCCCN1C=CN=C1	1	CICC1=CC(C(0)=0)=CC=
659	130224041510260217092803	2	MH ₂	NCC=C	10	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	m from	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	0C([C@H](C)CI)=0.[S]
660	130224041510260317022809	2	NH ₂	NCC=C	HO CO	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	····	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HOLOCI	CICC1=CC(C(O)=O)=CC=
661	130224041510260417032804	2	MH ₂	NCC=C	- ¹ 0^-	CIOC1=CC(C(O)=O)=CC=C1		CC(C)CCN	[™] r≁~	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO O S	0C([C@H](C)Cl)=0.[S]
662	130224041510260417032810	2	MH ₂	NCC=C	10	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	NUN CO	NCCC1=CC=C(OC)C(OC)=C1	HO O S	0C([C@H](C)CI)=0.[S]
663	130224051501260817022803	2	HIN CLO	NCC1=CC=C(OCO2)C	2 10	CICC1=CC(C(O)=O)=CC=C1	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HN	NCCCN1C=CN=C1	HO	CICC1=CC(C(O)=O)=CC=

664	130224051501260817022804	2		NCC1=CC=C(OCO2)C	но	ACIO(A1)-smiles CICC1=CC(C(O)=O)=CC=C1		Amines(A2)-smiles N[C@@H](C)C1=CC=CC=C1		Acid(X2)-smiles OC(C1=CSC(CCI)=N1)=0	H ₂ N 0	Amines(A3)-smiles NCC1=CC=CO1	но Станала	CICC1=CC(C(O)=O)=CC=
665	130224051502260317032802	2	H _A N CLO	NCC1=CC=C(OCO2)C	но	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(OCI)=N1)=O	H ₂ N	NCCO	HO S	OC([C@H](C)Cl)=0.[S]
666	130224061502260317032809	2	H _M CC	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)CI)=O.[S]
667	130224051502260417042808	2		NCC1=CC=C(OCO2)C:	но	CICC1=CC(C(O)=O)=CC=C1	H _N H _N	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H _A N Constant	BrC1=CC=C(CN)C=C1	HO O R	OC([C@H](C)Br)=O.[R]
668	130224061502260517092804	2	H _A N CLO	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	~О	CCC(O)=O
669	130224061502260817012803	2	H _A N CLO	NCC1=CC=C(OCO2)C	HO ^L OTO	CICC1=CC(C(O)=O)=CC=C1		N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H.M.~~N_ON	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
670	130224061503260317012803	2	H,M CLO	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HAR	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
671	130224051503260317022808	2	H _N N	NCC1=CC=C(OCO2)C	HO ^L OCO	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1	o= OH CI	OC(C1=COC(CCI)=N1)=O	H ₂ NBr	BrC1=CC=C(CN)C=C1	но	CICC1=CC(C(O)=O)=CC=
672	130224061503260317102804	2	H _A N CLO	NCC1=CC=C(OCO2)C.	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N ₄ s	N(C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)OC=C1
673	130224051503260517082803	2	HIN	NCC1=CC=C(OCO2)C.	HO ^L CCCO	CICC1=CC(C(O)=O)=CC=C1	H ₂ N / OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)Cl)=O.[S]
674	130224051503260717032802	2	HAN	NCC1=CC=C(OCO2)C.	Ho ¹ CCC	CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H _z N OH	NCCO	HO S	OC([C@H](C)Cl)=0.[S]
675	130224051503260817022801	2	H,N C	NCC1=CC=C(OCO2)C	ноборого	CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O		NCCC1=CNC2=CC=CC=C21	HOLOCO	CICC1=CC(C(O)=O)=CC=
676	130224051503261017092804	2	H,N	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(O)=O)=CC=C1	H,M^	NCC1=CC=C(CI)C=C1	m land	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]	∩О ОН	CCC(O)=O
677	130224051504260617102804	2	HAN	NCC1=CC=C(OCO2)C	но	CICC1=CC(C(0)=0)=CC=C1	NH ₂	NOC1=CC=CC=C1		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
678	130224051504260717032805	2	H _M CCC	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(0)=0)=CC=C1	A CANH	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NCC1COC(C=CC=C2)=C2O1	S S	OC([C@H](C)CI)=O.[S]
679	130224051504260917032803	2	H _M N	NCC1=CC=C(OCO2)C	но	CICC1=CC(C(0)=0)=CC=C1	nor of t	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HANNA	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
680	130224051504260917042803	2	HAN	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(O)=O)=CC=C1	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H,H ~ H / H	NCCON1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
681	130224051504261017032810	2	H _M N	NCC1=CC=C(OCO2)C	но	CICC1=CC(C(O)=O)=CC=C1	H _M A	NCC1=CC=C(CI)C=C1	₩ ¹ Υγγα	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)CI)=0.[S]
682	130224051509260217012803	2	H _M N	NCC1=CC=C(OCO2)C	но	CICC1=CC(C(O)=O)=CC=C1	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O	HJN YY	NCCCN1C=CN=C1	o= ↓ CI	OC(C1=CSC(CCI)=N1)=O
683	130224051509260217032802	2	HAN	NCC1=CC=C(OCO2)C	HO ^L COCO	CICC1=CC(C(O)=O)=CC=C1	w	NOC1=CC=CC(C(F)(F)F)=C1	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
684	130224051510260317032808	2	H _M CL	NCC1=CC=C(OCO2)C	HO ^L	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	HO TTO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N Br	BrC1=CC=C(CN)C=C1	HO O S	OC([C@H](C)CI)=O.[S]
685	130224051510260417022809	2	H,N C C C	NCC1=CC=C(OCO2)C	"	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	™¹tri∩ a	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HO I CO	CICC1=CC(C(O)=O)=CC=
686	130224051510260417032805	2	H _M N	NCC1=CC=C(OCO2)C	но	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	₩ ¹ ₩ ¹ Υ ^α	CIC/C(C)=C/[C@@H](C)C(O)=O	H _L N Y	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=0.[S]
687	130224061504260517102804	2	H ₂ N	NCC1=CC=CO1	"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC(C)(C)O	°↓↓↓ OH	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	of the	0=C(0)C1=C(C)0C=C1
688	130224071501260317022810	2	NH ₂	NCC1=CC=C(C)C=C1	Hold Contraction	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	N/ Co	NCCC1=CC=C(OC)C(OC)=C1	Ho ¹ C) a	CICC1=CC(C(O)=O)=CC=
689	130224071501260317032802	2	NH ₂	NCC1=CC=C(C)C=C1	HO ^L CO ^{CO}	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1	o=↓ OH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	0C([C@H](C)CI)=0.[S]
690	130224071501260917022809	2	NH ₂	NCC1=CC=C(C)C=C1	HO ^L CO ^{CO}	CICC1=CC(C(O)=O)=CC=C1	HAN TOT	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO ^L	CICC1=CC(C(0)=0)=CC=
691	130224071501261017022809	2	NH ₂	NCC1=CC=C(C)C=C1	Hold Contraction	CICC1=CC(C(O)=O)=CC=C1	H _A N ^A CO _{CI}	NCC1=CC=C(CI)C=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CC0CC1	Ho ¹	CICC1=CC(C(O)=O)=CC=
692	130224071502260217032802	2	NH ₂	NCC1=CC=C(C)C=C1	HO ^L COTO	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=O)(C)=O)C=C	J N CI	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	0C([C@H](C)CI)=0.[S]
693	130224071502260217032803	2	NH ₂	NCC1=CC=C(C)C=C1		CIOC1=CC(C(O)=O)=CC=C1	HAN COL	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	1.11 ~ 1 <u>0</u> 1	NCCON1C=CN=C1	HO S	OC([C@H](C)Cl)=0.[S]
694	130224071502260417032803	2	NH ₂	NCC1=CC=C(C)C=C1	<u>~</u> i ₀ ~	CICC1=CC(C(O)=O)=CC=C1	H_N ~~ ^H _Y ⁰	NCCNC(C)=0		0C(C1=CC=C(CCI)C=C1)=0	H.N.~~N	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=0.[S]
695	130224071502260717012808	2	NH ₂	NGC1=CC=C(C)C=C1	HO ^L	CIDC1=CC(C(0)=0)=CC=C1	A NHI	NOC1=CC=C(N(C)C)C=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N Br	BrC1=CC=C(CN)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
696	130224071502260817022803	2		NCC1=CC=C(C)C=C1	HOLOCA	CIOC1=CC(C(O)=O)=CC=C1	NH ₂	N[C@@H](C)C1=CC=CC=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	HAN NON	NCCON1C=CN=C1	Ho ¹	CICC1=CC(C(0)=0)=CC=

observation 697	full.mol.code2 130224071503260417102804	2	S Amines(X1)	Amines(X1)-smiles NCC1=CC=C(C)C=C1		Acid(X1)-smiles CICC1=CC(C(O)=O)=CC=C1		Amines(X2)-smiles NCCNC(C)=0		Acid(X2)-smiles OC(C1=CC=C(CCI)C=C1)=O	Amines(X3)	Amines(X3)-smiles N[C@@H](C)C1=CC=CC=C1.[S	Structure of Pair	Pair3.Acids O=C(O)C1=C(C)OC=C1
698	130224071503260817022803	2	NH ₂	NCC1=CC=C(C)C=C1	····	CICC1=CC(C(O)=O)=CC=C1	\mathbf{Q}	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	~ ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1	Holy a	CICC1=CC(C(O)=O)=CC=
699	130224071503260917022803	2	NH ₂	NCC1=CC=C(C)C=C1	HO TO A	CICC1=CC(C(O)=O)=CC=C1	H,N T T	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H,M~~N_)N	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
700	130224071503261017032801	2	NH ₂	NCC1=CC=C(C)C=C1	***	CICC1=CC(C(O)=O)=CC=C1	**************************************	NCC1=CC=C(CI)C=C1	OH HO ^L LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	Bar	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=O.[S]
701	130224071504260817012806	2	NH ₂	NCC1=CC=C(C)C=C1	HO TO TO	CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O		NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
702	130224081501260417032802	2		N1CONCCC1		CICC1=CC(C(O)=O)=CC=C1		NCCNC(C)=0	oH Carlor (OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HU S	OC([C@H](C)Cl)=0.[S]
703	130224081501260817022806	2	HN	N1CONCCC1	10	CICC1=CC(C(O)=O)=CC=C1	$\mathbf{\hat{\mathbf{P}}}$	N(C@@H)(C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O		NC[C@H](C)C1=CC=CC=C1	но	CICC1=CC(C(0)=0)=CC=
704	130224081501260817042803	2		N1CONCCC1		CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O		NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
705	130224081504260417092804	2		N1CONCCC1	10 L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H ^N ^O	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	CCC(O)=O
706	130224081504260517032802	2		N1CONCCC1		CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=0.[S]
707	130224081504260817092804	2		N1CONCCC1		CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН ОН	CCC(O)=O
708	130224081504260917042803	2	HN	N1CCNCCC1	HO CO	CICC1=CC(C(O)=O)=CC=C1	NALL A	NGC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	1,1 ~ 1 ₀ 1	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=0.[R]
709	130224081509260217042805	2	HN	N1CCNCCC1	10 × 10 × 0	CICC1=CC(C(O)=O)=CC=C1	HUR DEL	NCC1=CC=CC(C(F)(F)F)=C1	Holy a	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ⁻	NCC1COC(C=CC=C2)=C2O1	HO O R	OC([C@H](C)Br)=O.[R]
710	130224081509260317032810	2	HN	N1CONCCC1	10	CICC1=CC(C(O)=O)=CC=C1	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=0.[S]
711	130224091501260317012803	2	H ₂ N N	NCCCN1C=CN=C1	10 L	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(OCI)=N1)=O	H.H.~~YYH	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
712	130224091501260617032802	2	H ₂ H ~ N N	NCOCN1C=CN=C1	10	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1	€ Cutor	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
713	130224091501260717042802	2	H ₂ H	NCCCN1C=CN=C1	10 1 0 0	CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O R	OC([C@H](C)Br)=O.[R]
714	130224091501261017022809	2	H ₂ N N	NCCCN1C=CN=C1	10	CICC1=CC(C(O)=O)=CC=C1	H _M N	NCC1=CC=C(CI)C=C1	HO I TAY O	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
715	130224091501261017032805	2	H ₂ H ~~ N C N	NCCCN1C=CN=C1	10 1 0 0	CICC1=CC(C(O)=O)=CC=C1	HJN	NCC1=CC=C(CI)C=C1	HO LING	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=0.[S]
716	130224091501261017092804	2	H ₂ H M	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	H _N N C	NCC1=CC=C(CI)C=C1	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	⁰ ₀н	CCC(O)=O
717	130224091502260217012803	2	H ₂ H~N	NCCCN1C=CN=C1	HO LOTO	CICC1=CC(C(O)=O)=CC=C1	"	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	1.x~101	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
718	130224091502260317042803	2	Hall Market and All All All All All All All All All Al	NCCCN1C=CN=C1	" ^l U"	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O		NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
719	130224091502260617032809	2	H ₂ H~~~N~N	NCCCN1C=CN=C1	HO CON	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1	€ C	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=O.[S]
720	130224091502260717022802	2	H ₂ N~~N ₂ N	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	но	CICC1=CC(C(O)=O)=CC=
721	130224091502260717092804	2	н,н	NCCCN1C=CN=C1	10	CICC1=CC(C(O)=O)=CC=C1	Å.	NCC1=CC=C(N(C)C)C=C1	OF OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
722	130224091502260817022804	2	H ₂ N~~N ₂ N	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=C1	Real Real Provide Action of the second secon	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	но	CICC1=CC(C(0)=0)=CC=
723	130224091503260217032802	2	H ₂ N~~N_N	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
724	130224091503260417032807	2	ни	NCCCN1C=CN=C1	""	CICC1=CC(C(O)=O)=CC=C1	H ₂ N~ ^H / ^O	NCCNC(C)=O		0C(C1=CC=C(CCI)C=C1)=0		NCC1=CC(OC)=CC(OC)=C1	HO S	OC([C@H](C)Cl)=0.[S]
725	130224091503260617032802	2	ним	NCCCN1C=CN=C1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=C1	NH ₂	NOC1=CC=CC=C1	€ Contraction of the second se	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
726	130224091503260717042803	2	ни	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	11,11~~~1 ₁)1	NCCCN1C=CN=C1	HO O Br R	0C([C@H](C)Br)=0.[R]
727	130224091503261017032802	2	ным	NCCCN1C=CN=C1	<u>~</u> 10~	CICC1=CC(C(O)=O)=CC=C1	HyN	NCC1=CC=C(CI)C=C1	₩ ⁻¹ ₩ ⁻¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ~~OH	NCCO	HO C S	0C([C@H](C)CI)=0.[S]
728	130224091504260717032802	2	H ₂ H	NCOCN1C=CN=C1	HO LOTO	CICC1=CC(C(O)=O)=CC=C1	- AL	NOC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCCO	HO S	OC([C@H](C)CI)=O.[S]
729	130224091509260117032801	2	H ₂ N N	NCCCN1C=CN=C1	HO ^Î	CICC1=CC(C(O)=O)=CC=C1	nyr Cyfr	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	нл	NCCC1=CNC2=CC=CC=C21	HO. O S	CC([C@H](C)CI)=O.[S]

observation 730	full.mol.code2 130224091509260417012809	copies 2	Amines(X1)	Amines(X1)-smiles NCCCN1C=CN=C1	Acid(X1)	Acid(X1)-smiles CICC1=CC(C(O)=O)=CC=C1	Amines(X2)	Amines(X2)-smiles NCC1=CC=CC(C(F)(F)F)=C1	Acid(X2)	Acid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines(X3)	Amines(X3)-smiles NCC1CCOCC1	Structure of Pair	Pair3.Acids OC(C1=CSC(CCI)=N1)=O
			H,H		HO TOTO		HUN		HO TOTA	erere(e) efe@@rite)e(e) e	H ₂ N		ord rel ⊘H	
731	130224091509260417022802	2	нистр	NCCCN1C=CN=C1	HO CON	CICC1=CC(C(O)=O)=CC=C1	HAR CONT	NCC1=CC=CC(C(F)(F)F)=C1	····l	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	но	CICC1=CC(C(O)=O)=CC=
732	130224091509260417022809	2	ни	NCCCN1C=CN=C1	"	CICC1=CC(C(O)=O)=CC=C1	w	NCC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HOLOCA	CICC1=CC(C(O)=O)=CC=
733	130224091510260117092804	2	nn n>n	NCCCN1C=CN=C1	HO CO	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	H,N R	N[C@H](C)C1=CC=CC=C1.[R]	-~О ОН	CCC(O)=O
734	130224101501260217032802	2	HN	C1CNCCN1	HO LOT O	CICC1=CC(C(O)=O)=CC=C1	the second se	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
735	130224101501260317032802	2	HN	C1CNCCN1	10	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		0C(C1=C0C(CCl)=N1)=0	H ₂ N OH	NCCO	HU U S	OC([C@H](C)Cl)=O.[S]
736	130224101501260317042804	2	HN	C1CNCCN1	10	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		0C(C1=C0C(CCI)=N1)=0	H ₂ N	NCC1=CC=CO1	HO CO R	OC([C@H](C)Br)=O.[R]
737	130224101501260517032805	2	HN	C1CNCCN1	HO LOTO	CICC1=CC(C(O)=O)=CC=C1	H ₂ N OH	NCC(C)(C)O	ortical diamaterial diamateria anatorial diamaterial diamaterial diamaterial diamaterial diamaterial diamaterial diamaterial diamaterial diamat	0C(C1=CC=C(CCI)C=C1)=0	HUN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=O.[S]
738	130224101501260717032802	2	HN	C1CNCCN1	10	CICC1=CC(C(O)=O)=CC=C1	A Carner,	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
739	130224101502260417012802	2	HN	C1CNCCN1	10	CICC1=CC(C(O)=O)=CC=C1	H,N~H~O	NCCNC(C)=0		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO		OC(C1=CSC(CCI)=N1)=O
740	130224101502260417032804	2	HN	C1CNCCN1	10	CICC1=CC(C(0)=0)=CC=C1	H,N N YO	NCCNC(C)=0	• ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCC1=CC=CO1	HO C S	OC([C@H](C)Cl)=O.[S]
741	130224101502260717012803	2	HN	C1CNCCN1		CICC1=CC(C(O)=O)=CC=C1	A Com	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H,H ~~ 10/1	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
742	130224101502260717032802	2	HN	C1CNCCN1	10 × 10	CICC1=CC(C(O)=O)=CC=C1	-L.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N ^{OH}	NCCO	HO S	OC([C@H](C)CI)=O.[S]
743	130224101502260717032804	2	HN	C1CNCCN1	HO LOTO	CICC1=CC(C(O)=O)=CC=C1	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)CI)=O.[S]
744	130224101502260917032810	2	HN	C1CNCCN1	10 Long	CICC1=CC(C(O)=O)=CC=C1	HUN TO Y	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HAR COLOR	NCCC1=CC=C(OC)C(OC)=C1	IIO S	OC([C@H](C)CI)=O.[S]
745	130224101503260317032805	2	HN	C1CNCCN1	HO CON	CICC1=CC(C(O)=O)=CC=C1	H ₂ N	NCC1=CC=CS1		0C(C1=COC(CCI)=N1)=0	HAN	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)CI)=O.[S]
746	130224101503260617022803	2	HN	C1CNCCN1	*******	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1		0C(C1=CC=C(CCI)C=C1)=0	"" "	NCCCN1C=CN=C1	HO ^Î () ⁽	CICC1=CC(C(O)=O)=CC=
747	130224101503260917022809	2	HN	C1CNCCN1	HO CON	CICC1=CC(C(O)=O)=CC=C1	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=0	H,N O	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
748	130224101504260217022802	2	HN	C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1	NA CON	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N ^{OH}	NCCO	HO ^L	CICC1=CC(C(O)=O)=CC=
749	130224101504260417032802	2	HN	C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1	H _N N	NCCNC(C)=0	OH CO	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
750	130224101504260617102804	2	HN	C1CNCCN1	HO CON	CICC1=CC(C(O)=O)=CC=C1	NH ₂	NCC1=CC=CC=C1	°↓↓↓↓↓	0C(C1=CC=C(OCI)C=C1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	o → → OH	O=C(O)C1=C(C)OC=C1
751	130224101504260717032802	2	HN	C1CNCCN1	" ^l "	CICC1=CC(C(O)=O)=CC=C1	-horan	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N ^{OH}	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
752	130224101504260817042805	2	HN	C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HLN	NCC1COC(C=CC=C2)=C2O1	HO O R	OC([C@H](C)Br)=O.[R]
753	130224101504260917092802	2	HN NH	C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1	HUN TO T	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	но	CICC1=CC(C(O)=O)=CC=
754	130224101504260917092804	2	HN	C1CNCCN1	10	CICC1=CC(C(O)=O)=CC=C1	HAN TO Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
755	130224101509260117012803	2	HN	C1CNCCN1		CICC1=CC(C(O)=O)=CC=C1	w	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	ни	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
756	130224101509260117022801	2	HN	C1CNCCN1	10	CICC1=CC(C(O)=O)=CC=C1	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCC1=CNC2=CC=CC=C21	но	CICC1=CC(C(O)=O)=CC=
757	130224101509260217022803	2		C1CNCCN1	" ⁰	CICC1=CC(C(O)=O)=CC=C1	HAIL CONTRACT	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	11,10~~10 ⁰ 1	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
758	130224101509260417102802	2		C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1	w	NOC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	но	CICC1=CC(C(O)=O)=CC=
759	130224101510260317022809	2	HN	C1CNCCN1	"	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	HO LING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CC0CC1	HOLOCI	CICC1=CC(C(O)=O)=CC=
760	130224101510260417032801	2	HN	C1CNCCN1	<mark>ل</mark> ن~.	CICC1=CC(C(O)=O)=CC=C1		CC(C)CCN	[™] ÎŢ [*] ↑ [~] °	CIC/C(C)=C/[C@@H](C)C(O)=O	H _M N	NCCC1=CNC2=CC=CC=C21	HO C S	OC([C@H](C)Cl)=O.[S]
761	130324021501260417102804	2	H ₂ N	NCC1=CC=CN=C1		OC(C1=CSC(CCI)=N1)=O	H_N ~ H_O	NCCNC(C)=0	°↓↓↓↓↓	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
762	130324021501260617032801	2	H ₂ N	NCC1=CC=CN=C1	OH OH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	°↓))))))))))))))))))))))))))))))))))))	0C(C1=CC=C(CCI)C=C1)=0	H _M N	NCCC1=CNC2=CC=CC=C21	HO. O S	0C([C@H](C)CI)=0.[S]

observation 763	full.mol.code2 130324021502260417102804	2	H ₂ N	Amines(X1)-smiles NCC1=CC=CN=C1		Acid(X1)-smiles OC(C1=CSC(CCI)=N1)=O	Amines(X2)	Amines(X2)-smiles NCCNC(C)=O	Adid(X2)	Acid(X2)-smiles OC(C1=CC=C(CCI)C=C1)=O	Amines(X3)	Amines(X3)-smiles N[C@@H](C)C1=CC=CC=C1.[S	Structure of Pair OH	Pair3.Acids O=C(O)C1=C(C)OC=C1
764	130324021509260217092802	2	H ₂ N	NCC1=CC=CN=C1		OC(C1=CSC(CCI)=N1)=O	HUN C	NCC1=CC=CC(C(F)(F)F)=C1	····land	CIC/C(C)=C/[C@@H](C)C(O)=O	H,NY R	N(C@H)(C)C1=CC=CC=C1.[R]	HOLOCA	CICC1=CC(C(O)=O)=CC=
765	130324031501260217032802	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
766	130324031501260317032802	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NOC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
767	130324031501260517022802	2	H ₂ N~O	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	of the second	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	но	CICC1=CC(C(O)=O)=CC=
768	130324031502260217022803	2	H ₂ N~O~	NCCCOC		OC(C1=CSC(CCI)=N1)=O	HAN DO	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	····~··Di	NCCCN1C=CN=C1	HO ^Î (J [^])	CICC1=CC(C(O)=O)=CC=
769	130324031502260317032802	2	H ₂ N~O	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NOC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
770	130324031502260417012804	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H,N~~ ^H ~°	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N 0	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
771	130324031502260517032802	2	H ₂ N 0	NCCCOC		OC(C1=CSC(CCI)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO		OC([C@H](C)Cl)=O.[S]
772	130324031502260517032803	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H,H~~YY	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
773	130324031502260517092803	2	H ₂ N 0	NCCCOC		OC(C1=CSC(CCI)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	HO S	OC([C@H](C)Cl)=O.[S]
774	130324031502260917032805	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	NA CAR	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HUN	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=O.[S]
775	130324031503260417012803	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H,N~H~	NCCNC(C)=O	OH CI	0C(C1=CC=C(CCI)C=C1)=0	···^^_)	NCCON1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
776	130324031503260517012803	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC(C)(C)O	of the second se	OC(C1=CC=C(CCI)C=C1)=O	HAN NON	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
777	130324031503260617012803	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	o Canada	OC(C1=CC=C(CCI)C=C1)=O	H.H.~~Y_YH	NCCON1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
778	130324031504260417022806	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H,N H PO	NCCNC(C)=O	of the second se	OC(C1=CC=C(CCI)C=C1)=O	NH2	NC[C@H](C)C1=CC=CC=C1	но	CICC1=CC(C(O)=O)=CC=
779	130324031504260417032801	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H _A N~ ^H + ^O	NCCNC(C)=0	O CIT	OC(C1=CC=C(CCI)C=C1)=O	H,JI Contraction	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)CI)=0.[S]
780	130324031504261017012803	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H _A N ^A CA _O	NCC1=CC=C(CI)C=C1	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M~~N_)H	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
781	130324031504261017022803	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O	H _A N ^A CA _{CI}	NCC1=CC=C(CI)C=C1	no la porto	CIC/C(C)=C/[C@@H](C)C(O)=O	HUI YO	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
782	130324031509260117022809	2	H ₂ N	NCCCOC	C C C C C C C C C C C C C C C C C C C	OC(C1=CSC(CCI)=N1)=O	HALL Y	NCC1=CC=CC(C(F)(F)F)=C1	₩ ¹ 4~	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HO ^Î () ()	CICC1=CC(C(O)=O)=CC=
783	130324031509260217022809	2	H ₂ N O	NCCCOC		OC(C1=CSC(CCI)=N1)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
784	130324031509260217032802	2	H ³ N.~~^O~	NCCCOC		OC(C1=CSC(CCI)=N1)=O	w~QX	NCC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N [^] OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
785	130324031509260217042804	2	H ₂ N O	NCCCOC		OC(C1=CSC(CCI)=N1)=O	HAN CON	NOC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO O R	OC([C@H](C)Br)=O.[R]
786	130324031509260217092804	2	H ₂ N O	NCCCOC		OC(C1=CSC(CCI)=N1)=O	HUNTY'	NOC1=CC=CC(C(F)(F)F)=C1	₩ ¹ ₩	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
787	130324031509260317032805	2	H ₂ N O	NCCCOC	OH OH	OC(C1=CSC(CCI)=N1)=O	NUN C	NCC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	Hall	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=O.[S]
788	130324031509260417042803	2	H ₂ N O	NCCCOC		OC(C1=CSC(CCI)=N1)=O	with	NOC1=CC=CC(C(F)(F)F)=C1	₩ ¹ Υ ⁺	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N~~N_)N	NCCCN1C=CN=C1	HO O Br R	0C([C@H](C)Br)=0.[R]
789	130324031510260117012803	2	H ₂ N O	NCCCOC		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M ~ M _ M	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
790	130324031510260317032802	2	H ₂ N	NCCCOC		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	₩ ¹	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=0.[S]
791	130324041501260217092804	2	MH ₂	NCC=C	J N OH	OC(C1=CSC(CCI)=N1)=O	***	NOC1=CC=C(S(=O)(C)=O)C=C	CH CI	OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
792	130324041503260317092804	2	NH ₂	NCC=C	OF OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
793	130324041503260417022803	2	MH _z	NCC=C		OC(C1=CSC(CCI)=N1)=O	H2N ~~- ^H TO	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	HJN ~~ N_C)+	NCCCN1C=CN=C1	¹ 0^-	CICC1=CC(C(O)=O)=CC=
795	130324041504260417032801	2	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	H_N N YO	NCCNC(C)=0	of the second	0C(C1=CC=C(CCI)C=C1)=0	H _L N	NCCC1=CNC2=CC=CC=C21	HO O S	0C([C@H](C)CI)=0.[S]
796	130324041504260617092804	2	/NH ₂	NCC=C	O= OH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	of the second	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O

797	130324041504260717032802	2	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO		CC([C@H](C)CI)=O.[S]
798	130324041509260117022803	2	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1	······	CIC/C(C)=C/[C@@H](C)C(O)=O	HA YON	NCCCN1C=CN=C1	HOLOCA	CICC1=CC(C(O)=O)=CC=
799	130324041509260117032803	2	MH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	NAN CONT	NOC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N M	NCCCN1C=CN=C1	HO O S	0C([C@H](C)CI)=0.[S]
800	130324041509260317032803	2	NH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	HAN CONT	NOC1=CC=CC(C(F)(F)F)=C1	·····	CIC/C(C)=C/[C@@H](C)C(O)=O	ни~~~чСу	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
801	130324041509260417032801	2	MH ₂	NCC=C		OC(C1=CSC(CCI)=N1)=O	141 J	NCC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	нл	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=0.[S]
802	130324051501260217022802	2	H _A N CCO	NCC1=CC=C(OCO2)C	STAR	OC(C1=CSC(CCI)=N1)=O	****	NCC1=CC=C(S(=0)(C)=0)C=C	o	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HOLOCA	CICC1=CC(C(O)=O)=CC=
803	130324051501260217032802	2	HN CCO	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	"	NCC1=CC=C(S(=0)(C)=0)C=C	Q= CH	OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
804	130324051501260617012804	2	HIN CO	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1	O= OH	OC(C1=CSC(CCI)=N1)=O
805	130324051501260617032806	2	H,N CC O	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)CI)=O.[S]
806	130324051501260717032802	2	HÍN CLO	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	A CANH	NCC1=CC=C(N(C)C)C=C1	Q → CI	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
807	130324051501260817032810	2	HĮN CO	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	Real Real Provide American Science Provide Ame	N[C@@H](C)C1=CC=CC=C1	CI C	OC(C1=CSC(CCI)=N1)=O	RUN COLO	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)Cl)=0.[S]
808	130324051502260217032801	2	H ₂ N C C O	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C(S(=0)(C)=0)C=C	O → CI OH	OC(C1=COC(CCI)=N1)=O		NCCC1=CNC2=OC=CC=C21	HO S	ОС([C@H](C)Cl)=0.[S]
809	130324051502260617022809	2	H ₄ M	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	o to	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HOLOCA	CICC1=CC(C(O)=O)=CC=
810	130324051503260417012803	2	HIN	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	H,N~ ^H Y ^O	NCCNC(C)=0	ortication of the second seco	OC(C1=CC=C(CCI)C=C1)=O	HANNA	NCCCN1C=CN=C1	OH CI	OC(C1=CSC(OCI)=N1)=O
811	130324051503260617032802	2	H ₂ N C C C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCCO	S	OC([C@H](C)Cl)=0.[S]
812	130324051503260917022809	2	H ₂ N C C C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	HAR OF Y	NCC1=CC(F)=CC(C(F)(F)F)=C1	Q → CI OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CODCC1	HOLOCA	CICC1=CC(C(O)=O)=CC=
813	130324051504260617032808	2	H ₂ N C C C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	°↓↓↓ ⊂	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ⁻	BrC1=OC=C(CN)C=C1	HO S	OC([C@H](C)Cl)=O.[S]
814	130324051504260817102804	2	HĨN	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	Killer (N[C@@H](C)C1=CC=CC=C1	CI CH CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ₄ s	N[C@@H](C)C1=CC=CC=C1.[S	OH O	O=C(O)C1=C(C)OC=C1
815	130324051504260917012803	2	H ₂ N CC 0	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	NN YY	NCC1=CC(F)=CC(C(F)(F)F)=C1	Q → CI	OC(C1=CSC(CCI)=N1)=O	H.M.~~ N	NCCCN1C=CN=C1	OH CI	OC(C1=CSC(CCI)=N1)=O
816	130324051509260217092804	2	H ₂ N	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	en C	NOC1=CC=CC(C(F)(F)F)=C1	₩ ¹ Υ ⁴	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
817	130324051509260317032806	2	HJN CO	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	HAR CON	NCC1=CC=CC(C(F)(F)F)=C1	Hole to	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)CI)=O.[S]
818	130324051509260417022807	2	H,N C C C	NCC1=CC=C(OCO2)C		OC(C1=CSC(CCI)=N1)=O	w J	NCC1=CC=CC(C(F)(F)F)=C1	₩ ¹ ₩	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC(OC)=CC(OC)=C1	HOP I TO TO	CICC1=CC(C(O)=O)=CC=
819	130324061504260517032802	2	H ₂ N	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	°↓↓↓ ⊂	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
820	130324071501260217032802	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	~~~Q_{	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
821	130324071501260417032808	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N~ ^H + ^O	NCCNC(C)=O	ortica M	0C(C1=CC=C(CCI)C=C1)=0	H _A N	BrC1=OC=C(CN)C=C1	HO S	OC([C@H](C)CI)=O.[S]
822	130324071501260617032806	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	NH ₂	NCC1=CC=CC=C1	OH CON	0C(C1=CC=C(CCI)C=C1)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O S	0C([C@H](C)Cl)=0.[S]
823	130324071501260717032810	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	- Com	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HUMAN CON	NCCC1=CC=C(OC)C(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]
824	130324071502260317102804	2	NH ₂	NCC1=CC=C(C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	O O OH	OC(C1=COC(CCI)=N1)=O	H2N	N[C@@H](C)C1=CC=CC=C1.[S	OH O	0=C(0)C1=C(C)0C=C1
825	130324071502260517032802	2	NH ₂	NCC1=CC=C(C)C=C1	S CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC(C)(C)O	° ↓ ↓ ↓ ↓ ↓	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
826	130324071502260817102804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1	O-CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	o H	O=C(O)C1=C(C)OC=C1
827	130324071503260417032802	2	NH ₂	NCC1=CC=C(C)C=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	H2N ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ~-OH	NCCO	HO O S	0C([C@H](C)CI)=0.[S]
828	130324071503260517092803	2	NH ₂	NCC1=CC=C(C)C=C1	OF OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO S	OC([C@H](C)CI)=O.[S]
829	130324071503261017032802	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ^N C	NCC1=CC=C(CI)C=C1	HO ^L TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO. O S	oc([C@H](C)Cl)=0.[S]

830	130324071504260317042803	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H,M ~ (C)4	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
831	130324071504260417042806	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H _A N N YO	NCCNC(C)=0	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O R	OC([C@H](C)Br)=O.[R]
832	130324071504260517032803	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	HAI ~ 100	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
833	130324071504261017022803	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	HAN CO.	NCC1=CC=C(CI)C=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	w~~~vD	NCCCN1C=CN=C1	HO ¹ CCC	CICC1=CC(C(O)=O)=CC=
834	130324071509260417042804	2		NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O	HAR CON	NCC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO O R	OC([C@H](C)Br)=O.[R]
835	130324071510260117102804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	HOLE A	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N S	N(C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
836	130324071510260417032804	2	NH ₂	NCC1=CC=C(C)C=C1		OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	Holy of	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N O	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=O.[S]
837	130324081501260217032802	2		N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	HAN DE	NCC1=CC=C(8(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
838	130324081501260317032806	2		N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	NH2	NC[C@H](C)C1=CC=CC=C1	HO S	OC([C@H](C)Cl)=O.[S]
839	130324081501260617012803	2	HN	N1CONCCC1	S C C C C C C C C C C C C C C C C C C C	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(OCI)C=C1)=O	HN	NCCCN1C=CN=C1	O=OH	OC(C1=CSC(CCI)=N1)=O
840	130324081502260717012803	2	HN	N1CONCCC1	o= ↓ ∩ ⊂	OC(C1=CSC(CCI)=N1)=O	-La Maria	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HM-10	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
841	130324081503260217102804	2	HN	N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	"	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
842	130324081503260317032803	2	HN	N1CONCCC1	Q Q OH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CS1	o=↓ OH	OC(C1=COC(CCI)=N1)=O	···~~D	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
843	130324081503260617012803	2	HN	N1CONCCC1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	OH CI	OC(C1=CC=C(CCI)C=C1)=O	HAI~~YYI	NCCCN1C=CN=C1	O-CI	OC(C1=CSC(CCI)=N1)=O
844	130324081503260717092802	2		N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO ^Î ()	CICC1=CC(C(O)=O)=CC=
845	130324081503260717102804	2	HN	N1CCNCCC1		OC(C1=CSC(CCI)=N1)=O	-L	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH O	O=C(O)C1=C(C)OC=C1
846	130324081503260817032809	2		N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	C NH,	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO S	OC([C@H](C)CI)=O.[S]
847	130324081504260517032802	2	HN	N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	H ₂ N /	NCC(C)(C)O	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
848	130324081504261017102804	2		NICONCOCI		OC(C1=CSC(CCI)=N1)=O	H ₂ N ¹ Cl	NCC1=CC=C(CI)C=C1	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH O	O=C(0)C1=C(C)OC=C1
849	130324081509260217032807	2		NICONCCC1		OC(C1=CSC(CCI)=N1)=O	HALL I	NOC1=CC=CC(C(F)(F)F)=C1	₩ ¹ Υγγα	CIC/C(C)=C/[C@@H](C)C(O)=O	$\operatorname{Add}_{\operatorname{Add}}$	NCC1=CC(OC)=CC(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]
850	130324081509260217042803	2		N1CONCCC1		OC(C1=CSC(CCI)=N1)=O	HALL CAL	NCC1=CC=CC(C(F)(F)F)=C1	HO I FOI T	CIC/C(C)=C/[C@@H](C)C(O)=O	"" "	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
851	130324091501260217022809	2	н,п~~у~	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	"" " " " " " " " " " " " " " " " " " "	NCC1=CC=C(S(=0)(C)=0)C=C	CH CI	OC(C1=COC(CCI)=N1)=O	H,N O	NCC1CCOCC1	Hor ¹ Corro	CICC1=CC(C(O)=O)=CC=
852	130324091501260317092804	2	ни	NCOCN1C=GN=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	O= OH	OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
853	130324091501260717032802	2	н,н	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	-La Million	NCC1=CC=C(N(C)C)C=C1	o≓ OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
854	130324091501260917032805	2	н,н	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O	NUT Y	NCC1=CC(F)=CC(C(F)(F)F)=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ² C	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=O.[S]
855	130324091502260517032804	2	н,н	NCCCN1C=CN=C1	OF OH	OC(C1=CSC(CCI)=N1)=D		NCC1=CC=CC=C1	°↓↓↓ ∩	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)CI)=O.[S]
856	130324091502260717022806	2	н,н	NCCCN1C=GN=C1		OC(C1=CSC(CCI)=N1)=O	L. MIL	NCC1=CC=C(N(C)C)C=C1	orton orton	OC(C1=CSC(CCI)=N1)=0	NH,	NC[C@H](C)C1=CC=CC=C1	HO LOTO	CICC1=CC(C(0)=0)=CC=
857	130324091503260317042803	2	ним	NCCCN1C=CN=C1	O-CH	OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	o_ OH	OC(C1=COC(CCI)=N1)=O	"" "Di	NCCCN1C=CN=C1	HO O Br R	0C([C@H](C)Br)=0.[R]
858	130324091503260417012803	2	н,н	NCOCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	H _A N N YO	NCCNC(C)=O	°↓↓↓↓↓	OC(C1=CC=C(CCI)C=C1)=O	***~~D	NCCCN1C=CN=C1	→ → CI	OC(C1=CSC(CCI)=N1)=O
859	130324091503260717022803	2	ни	NCCCN1C=CN=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	- Com	NOC1=CC=C(N(C)C)C=C1	o=√H G	OC(C1=CSC(CCI)=N1)=O	"" "D"	NCCCN1C=CN=C1		CICC1=CC(C(0)=0)=CC=
860	130324091503260817012803	2	H,N N	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	NH,	N[C@@H](C)C1=CC=CC=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	HM ~~ 10	NCCCN1C=CN=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O
861	130324091503260817022809	2	ни	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O		N(C@@H)(C)C1=CC=CC=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H _J N	NCC1CCOCC1	HO LOCA	CICC1=CC(C(0)=0)=CC=
862	130324091504260317032805	2	ним	NCCCN1C=CN=C1	OH OH	OC(C1=CSC(CCi)=N1)=O	H ₂ N S	NCC1=CC=CS1	o	OC(C1=COC(CCI)=N1)=O	H,N	NCC1COC(C=CC=C2)=C2O1	HO. O S	OC([C@H](C)Cl)=0.[S]

863	130324091509260217102804	2		NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	HO LIVE)	ACID(X2)-3111169 CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N s	N[C@@H](C)C1=CC=CC=C1.[S		0=C(0)C1=C(C)0C=C1
864	130324091509260317022808	2	H ₂ N~N	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	HUN Y	NCC1=CC=CC(C(F)(F)F)=C1	"lysyn	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN DO	BrC1=CC=C(CN)C=C1	н	CICC1=CC(C(O)=O)=CC=
865	130324091509260417022806	2	H2N~~N~N	NCOCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O	www.t	NCC1=CC=CC(C(F)(F)F)=C1	n I	CIC/C(C)=C/[C@@H](C)C(O)=O		NC[C@H](C)C1=CC=CC=C1		CICC1=CC(C(O)=O)=CC=
866	130324091510260417102804	2	n,n ~~~ n ~ n	NCCCN1C=CN=C1	ост _{он}	OC(C1=CSC(CCI)=N1)=O		OC(C)CCN	" 1 1 °	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1.[S	C OH	O=C(O)C1=C(C)OC=C1
867	130324101501260217042801	2		C1CNCCN1	o≓(oH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C(S(=0)(C)=0)C=C ⁺		OC(C1=COC(CCI)=N1)=O	0	NCCC1=CNC2=CC=CC=C21	о́ то но ро	OC([C@H](C)Br)=O.[R]
868	130324101501260317032802	2		C1CNCCN1	O= OH	OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CS1	o= √H √	OC(C1=COC(CCI)=N1)=O		NCCO	HO O	OC/[C@H](C)CI)=O.[S]
869	130324101501260617012805	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O		NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
870	130324101501260917032802	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	`	NCCO		OC([C@H](C)Cl)=O.[S]
871	130324101501261017022805	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C(CI)C=C1	о= ОН	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1COC(C=CC=C2)=C2O1	s s	CICC1=CC(C(0)=0)=CC=
872	130324101501261017032805	2	HN	C1CNCCN1	OH OH	00(01=090(001=N1)=0	H ₂ M Cl	NOC1=CC=C/CIIC=C1	ноците	വവസ് പ്രത്യക്ഷി പ്രവസം പ		NGC1COC/C=CC=C2)=C2O1	HO TO	0C/[C@H](C)C)=0 [S]
		-	HN		O= OH		H,N C		HO TO		HAVE		HO S	
8/3	130324101502260317032807	2	HN	CTONCONT		OC(C1=CSC(OCI)=N1)=O	H ₂ N	NOC1=CC=CS1		0C(C1=C0C(CCI)=N1)=0	Υ, ^m	NGC1=CC(OC)=CC(OC)=C1	HO S	OC([C((BH)(C)CI)=0.[S]
874	130324101502260317042805	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HJN	NCC1COC(C=CC=C2)=C2O1	HO O R	OC([C@H](C)Br)=O.[R]
875	130324101502260417012803	2	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H ₂ N~ ^H +°	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=0	""^^D	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
876	130324101502260717032806	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	-L Colored	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)CI)=O.[S]
877	130324101502260817022804	2	HN	C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	\mathbf{Q}	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO ^L OCO	CICC1=CC(C(O)=O)=CC=
878	130324101502260817022809	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HJN	NCC1CCOCC1	He Land	CICC1=CC(C(O)=O)=CC=
879	130324101502260817032802	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	NH ₂	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
880	130324101503260317092802	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	* u	CICC1=CC(C(O)=O)=CC=
881	130324101503260717022802	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	4	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	н, м он	NCCO		CICC1=CC(C(O)=O)=CC=
882	130324101504260217022809	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=C(S(=0)(C)=0)C=C1	отон Сура	OC(C1=COC(CCI)=N1)=O	H _I N	NCC1CCOCC1	₩ ¹ γγα	CICC1=CC(C(O)=O)=CC=
883	130324101504260317012803	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
884	130324101504260317042803	2		C1CNCCN1		OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	o≓ _{OH}	OC(C1=COC(CCI)=N1)=O		NCCCN1C=CN=C1		OC([C@H](C)Br)=O.[R]
885	130324101504260817032802	2		C1CNCCN1	остон См	OC(C1=CSC(CCI)=N1)=O	\bigcirc	N[C@@H](C)C1=CC=CC=C1	ordon Gradina Gradin Gradina Gradina Gradina Gradina Gradina Gradina Gradina Gradina	OC(C1=CSC(CCI)=N1)=O		NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
886	130324101509260317022803	2		C1CNCCN1	o≓ oH	OC(C1=CSC(CCI)=N1)=O	NH2	NCC1=CC=CC(C(F)(F)F)=C1	о=< _{он}	CIC/C(C)=C/[C@@H](C)C(O)=O	HN	NCCON1C=CN=C1	i	CICC1=CC(C(O)=O)=CC=
887	130324101509260417022807	2		C1CNCCN1	o≓(oH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	** 1 ¶ °	CIC/C(C)=C/[C@@H](C)C(O)=O	~~~ [*]	NCC1=CC(OC)=CC(OC)=C1	i (j -	CICC1=CC(C(O)=O)=CC=
888	130324101510260417032804	2		C1CNCCN1	о= он	OC(C1=CSC(CCI)=N1)=O		CC(C)CCN	₩~¶~¶~a	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CO1	но фо	OC([C@H](C)CI)=O.[S]
889	130424011503260317022808	2		NCC1=CC=CC(Br)=C1	о= он	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O		BrC1=CC=C(CN)C=C1	× `	CICC1=CC(C(O)=O)=CC=
890	130424011503260617032802	2		NCC1=CC=CC(Br)=C1	****	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	and the second s	NCCO	H0	OC([C@H](C)Cl)=O.[S]
891	130424011504260317022803	2	HAN" T	NCC1=CC=CC(Br)=C1	Hotel a	CIC/C(C)=C/[C@@H](C)C(O)=O	C NH2	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=0	H ₂ N OH	NCCCN1C=CN=C1	s s	CICC1=CC(C(0)=0)=CC=
892	130424011504260317102804	2	H ₂ N Br	NCC1=CC=CC(Br)=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCi)=N1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S	HO ^L	0=C(0)C1=C(C)0C=C1
893	130424021502280212032802	2	H _k N	NCC1=CC=CN=C1	Holy Co	വാഗവ=വശക്ഷപ്പാഗം-റ	H ₂ N S	NOC1=CC=C/S/=01/C1=01/C		00(01=000(00%=N4%=0	₿ s	NCCO	• <u></u>	00/(00H)(0/01=0.191
004	200 40 400 45 000000	-	H ₂ N N		"T		*** C) ~		O=OH		H ₂ N ~~ OH		HO C S	
034	130424021503260817022803	2	H ₂ N	NGC1=CC=CN=C1		니나다(다)=나(다멙쉖H)(C)C(0)=0	Real Provided Action	NUBBEN(C)C1=CC=CC=C1	o=↓ OH	00(01=030(001)=N1)=0	HAI DI	NUGUNTU=CN=C1	Ho ¹	UKUT=CC(C(0)=0)=CC=
895	130424021504260317032803	2	H ₂ N	NCC1=CC=CN=C1	HO LING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1	o≓ OH CI	OC(C1=COC(CCI)=N1)=O	ни~~Di	NCCCN1C=CN=C1	HO- O S	OC([C@H](C)Cl)=O.[S]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair	Pair3.Acids
896	130424021509260417092804	2	H ₂ N	NCC1=CC=CN=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	in the	NOC1=CC=CC(C(F)(F)F)=C1	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
897	130424031501260217032802	2	H ₃ N~0	NCCCOC	····ly~	CIC/C(C)=C/[C@@H](C)C(O)=O	"``Q	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
898	130424031501260217032803	2	H ₂ N~0	NCCCOC	HO TOTA	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN COLOR	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H.M.~~V_M_M	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
899	130424031501260817032802	2	H ₂ N	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O	\mathbf{Q}	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HOOS	OC([C@H](C)Cl)=O.[S]
900	130424031501260917092804	2	H ₂ N~0~	NCCCOC	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	HAINTY'	NOC1=CC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
901	130424031501261017032809	2	H ₂ N~0~	NCCCOC	m la sera	CIC/C(C)=C/(C@@H)(C)C(O)=O	H,M Ca	NCC1=CC=C(CI)C=C1	ночерена	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HU S	OC((C@H)(C)Cl)=0.[S]
902	130424031502260117102802	2	H ₂ N	NCCCOC	Holy of	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N 0	NCCOC	∫ N ^a	OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S		CICC1=CC(C(O)=O)=CC=
903	130424031502260217032802	2	H ₂ N O	NCCCOC	Jan Strange	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN Q	NCC1=CC=C(8(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O		NCCO	HO S	OC([C@H](C)CI)=O.[S]
904	130424031502260217032810	2	H ₂ N~0~	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O	***	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O		NCCC1=CC=C(OC)C(OC)=C1		OC([C@H](C)Cl)=0.[S]
905	130424031502260617032806	2	H ₂ N~0~	NCCCOC		CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC=CC=C1	от он	OC(C1=CC=C(CCI)C=C1)=O		NC[C@H](C)C1=CC=OC=C1	HO O S	OC([C@H](C)Cl)=O.[S]
906	130424031502261017102803	2	HIN	NCCCOC	1 I	CIC/C(C)=C/[C@@H](C)C(O)=O	~ **^^	NCC1=CC=C(CI)C=C1	du la com	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ NH ₂	N[C@@H](C)C1=CC=CC=C1.[S	HO S	OC([C@H](C)CI)=O.[S]
907	130424031503260317032802	2		NCCCOC	lan.	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O		NCCO		OC([C@H](C)Cl)=0.[S]
908	130424031503260417092804	2	HN	NCCCOC	lan.	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=0	скон Сон	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]		CCC(O)=O
909	130424031503260517012803	2		NCCCOC	in 1 1 a	CIC/C(C)=C/[C@@H](C)C(O)=O	ОН	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O		NCCCN1C=CN=C1	он	OC(C1=CSC(CCI)=N1)=O
910	130424031503260617042802	2		NCCCOC	™¶¶™ Lutr	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	۳. ۱۳۰۰	OC(C1=CC=C(CCI)C=C1)=O	~ .0H	NCCO	о= он но_о	OC([C@H](C)Br)=O.[R]
911	130424031503261017042806	2		NCCCOC	P P	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=C(CI)C=C1	° Currona de la companya de la compa	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ² ~	NC[C@H](C)C1=CC=CC=C1	HO_O	OC([C@H](C)Br)=O.[R]
912	130424031504260617012803	2	H ⁵ N ² 0 ²	NCCCOC	HO~Y~~~~	CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NCCCN1C=CN=C1	Br R	OC(C1=CSC(CCI)=N1)=O
913	130424031504260817032802	2	H ₂ N	NCCCOC	*******	CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		CC(C1=CSC(CCI)=N1)=O	nn - Di	NCCO		OC([C@H](C)CI)=0.[S]
914	130424031509260217022802	2	H ₂ N 0	NCCCOC	"	CIC/C(C)=C/[C@@H](C)C(O)=O	KNH,	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	د م	CICC1=CC(C(O)=O)=CC=
915	130424031509260217022803	2	H ₂ N	NCCCOC	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN TOX	NOC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCCN1C=CN=C1	HO 100	CICC1=CC(C(0)=0)=CC=
916	130424031509260317012803	2	H ₂ N~0	NCCCOC	₩ ¹ ₩	CIC/C(C)=C/[C@@H](C)C(O)=O	HAUNDY.	NCC1=CC=CC(C(F)(F)F)=C1	₩ ¹ ¶~\~o	CIC/C(C)=C/[C@@H](C)C(O)=O	HN NON	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
917	130424031509260417012803	2	H ₂ N	NECCOC	HO TO	CIC/C(C)=C/(CB@H)(C)C(O)=0	HAN CON	NOC1=CC=CC(C(F)(F)F)=C1	HO TO	CIC/C/C)=C/IC@@H1/C)C(O)=O	HM - 104	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
918	130424031500280417012804	2	H ₂ N-~~	NCCCOC	HO TY O	CIC/C/2=C/C/2008H1/C/C/O/2=O	•••~DX	NOC1=0C=00(0(F)/F)=01	[™] ¹	00000=000000000	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC=CO1	OH CI	0C/C1=CSC/CCI)=N1)=0
210	130-240 1303200-1101200-	2	H ₂ N		HOTA	00000-010888000000-0	HAN CON		HO I TO		H ₂ N		O=OH	
919	130424031509260417012806	2	H ₂ N	NCCCOC	Holy to	CIC/CIC)=C/(CBBH)(C)C(O)=O	white the second	NGC1=CC=CC(C(F)(F)F)=C1	[™] ¹ γ~	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[OBH](C)C1=CC=CC=C1	O=CH	00(C1=CSC(0Cl)=N1)=0
920	130424031510260117102804	2	H ₂ N 0	NCCCOC	HO I TO	CIC/C(C)=C/(CB@H)(C)C(O)=O		CC(C)CCN	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
921	130424031510260317012806	2	H ₂ N	NCCCOC	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	"	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
922	130424031510260417042805	2	H ₂ N~0~	NCCCOC	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1COC(C=CC=C2)=C2O1	HO O R	OC([C@H](C)Br)=O.[R]
923	130424041501260317012805	2	NH ₂	NCC=C	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HJN	NCC1COC(C=CC=C2)=C2O1		OC(C1=CSC(CCI)=N1)=O
924	130424041501260417022807	2	NH ₂	NCC=C		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N N YO	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC(OC)=CC(OC)=C1	но	CICC1=CC(C(O)=O)=CC=
925	130424041501260517032806	2	NH ₂	NCC=C	no la proprio	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O		NC[C@H](C)C1=CC=OC=C1	HO S	OC([C@H](C)Cl)=0.[S]
926	130424041501260517102804	2	// NH ₂	NCC=C	"	CIC/C(C)=C/[C@@H](C)C(0)=0	H ₂ N	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	Hand	N(C@@H)(C)C1=CC=CC=C1.[S	o H	O=C(O)C1=C(C)OC=C1
927	130424041502260617022802	2	MH ₂	NCC=C	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	₩ ¹	CICC1=CC(C(O)=O)=CC=
928	130424041502260717022803	2	NH ₂	NCC=C	но	CIC/C(C)=C/[C@@H](C)C(O)=O	A Que	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=0	HM 104	NCCCN1C=CN=C1	HO ¹ CT CI	CICC1=CC(C(O)=O)=CC=
									OH					

observation 929	full.mol.code2 130424041503260217032802	2	Amines(X1)	Amines(X1)-smiles NCC=C	Acid(X1)	Acid(X1)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	Amines(X2)	Amines(X2)-smiles NCC1=CC=C(S(=O)(C)=O)C=C*	Acid(X2)	Acid(X2)-smiles OC(C1=COC(CCI)=N1)=O	Amines(X3)	Amines(X3)-smiles NCCO	Structure of Pair	Pair3.Acids OC([C@H](C)Cl)=O.[S]
			MH ₂		The second se		~ V,		C→ N		H ₂ N OH		s s	
930	130424041503260417032802	2	NH ₂	NCC=C	100 Lange - 0	CIC/C(C)=C/[C@@H](C)C(O)=O	H _N N	NCCNC(C)=O	°↓ Chi	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
931	130424041509260117032808	2	MH ₂	NCC=C	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	ни	NCC1=CC=CC(C(F)(F)F)=C1	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	BrC1=CC=C(CN)C=C1	HO S	OC([C@H](C)Cl)=O.[S]
932	130424041510260417012803	2	NH ₂	NCC=C	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	HON THE ACT	CIC/C(C)=C/[C@@H](C)C(O)=O	***~~~*D	NCCCN1C=CN=C1	o= OH	OC(C1=CSC(CCI)=N1)=O
933	130424051501260217012809	2	H _A N C C O	NCC1=CC=C(OCO2)C	"	CIC/C(C)=C/[C@@H](C)C(O)=O	***	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCCCC1	O= OH	OC(C1=CSC(CCI)=N1)=O
934	130424051501260717022803	2	H,N C C O	NCC1=CC=C(OCO2)C	no la francia	CIC/C(C)=C/(C@@H)(C)C(O)=O	A Com	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	HAI ~ HOI	NCCCN1C=CN=C1	HO ^L	CICC1=CC(C(O)=O)=CC=
935	130424051501260717022809	2	H,N C C O	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	A AM	NOC1=CC=C(N(C)C)C=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	HO LOTO	CICC1=CC(C(0)=0)=CC=
936	130424051502260417032806	2	H _A N CCO	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	H,N N YO	NCCNC(C)=0		0C(C1=CC=C(CCI)C=C1)=0	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO O S	OC([C@H](C)CI)=O.[S]
937	130424051503260417042803	2	H _A N CCC	NCC1=CC=C(OCO2)C	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N H ² N H ² N	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=0	HM ~~ 104	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
938	130424051503260717032802	2	HÍN	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	A CANH,	NCC1=CC=C(N(C)C)C=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
939	130424051504260317032803	2	HAN	NCC1=CC=C(OCO2)C		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1	orten de la contra de la contr	OC(C1=COC(CCI)=N1)=O	HAI ~ 10	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
940	130424051509260117032801	2	H _A N O	NCC1=CC=C(OCO2)C	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAN	NOC1=OC=CC(C(F)(F)F)=C1	HO I TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H _M N	NCCC1=CNC2=CC=CC=C21	HO O S	0C([C@H](C)CI)=0.[S]
941	130424051510260217032805	2	H_N O	NCC1=CC=C(OCO2)C	"	CIC/C(C)=C/(C@@H)(C)C(O)=O		CC(C)CCN	Hold Table	CIC/C(C)=C/(C@@H)(C)C(O)=O	H _N N	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)CI)=0.[S]
942	130424061501260217102804	2	H ₂ N	NCC1=CC=CO1	₩ ¹	CIC/C(C)=C/(CB(BH)(C)C(O)=O	M Of	NOC1=CC=C(S(=O)(C)=O)C=C'		OC(C1=COC(CCI)=N1)=O	HAN S	N[C @ @H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
943	130424061501260717022809	2	H ₂ N	NCC1=CC=CO1	₩ ¹	CIC/C(C)=C/(C@@H)(C)C(O)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=0	H ₂ N		HO ^Î () ()	CICC1=CC(C(0)=0)=CC=
944	130424061504260317032803	2	H ₂ N	NCC1=CC=CO1	₩ ¹ τγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγγ	CIC/C(C)=C/(CB(BH)(C)C(O)=O	H ₂ N	NOC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	ни	NCCON1C=CN=C1	HO S	OC([C((()())])(C)(C))=0.[S]
940	1304240/150126021/012803	2	NH ₂	NUC1=UC=U(U)U=U1	HO TO		"	NGC1=CC=C(S(=0)(C)=C)C=C			1.01 mg/		o= OH	
946	130424071501260317032802	2	NH ₂	NGC1=GG=G(G)G=G1	₩ ¹	00000-0108841(0)0(0)=0	H ₂ N	NGC1=CC=CS1		00(01=000(00)=N1)=0	H ₂ N OH	NGCO	HO S	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
040	100424071001200717022000	2			HO I TO		A A A A A A A A A A A A A A A A A A A				HAN		HO LOTO	
040	1304240/150126091/032808	2	NH ₂	NCC1=CC=C(C)C=C1	HO TO		HAN TOT	NOC1=00(F)=00(0(F)(F)(F)=01			H _N		HO C S	00((0@H)(0)0)=0.[5]
343	130424071301201017032803	2	NH ₂	NUC	HO TO		H/M CO		HO TY O		1.VI ~ 101		HO O S	
950	130424071502260517022810	2	NH ₂		HOLING		H ₂ N OH				HIM CO		" ^Î UT"	
901	1304240/1502260/17/022803	2	NH ₂	NUC1=UC=U(U)U=U1	Hort to			NGC1=CC=C(N(C)C)C=C1			1.51 ~ 1/2 1 1/2 1		HO ^Î	
952	130424071502260817022804	2	NH ₂	NCC1=CC=C(C)C=C1	HO TY O	CCC(C)=C1(CB@H)(C)C(O)=O		N[C@@H](C)C1=CC=CC=C1	ortor CH	00(C1=CSC(CCI)=N1)=0	H ₂ N	NCC1=CC=CO1	HO ^Î () ()	00001=00(0(0)=0)=00=
803	13042407 150225 1017 022803	2	NH ₂		HO I TO		H,M CO		HOLY		HAI ~ 10	NOCONIC=CN=C1	HO LOTO	
204	13042407 13032604 17022603	2	NH ₂		HO TO		H,N ~ H ~ O				***~~Y		HO LOTO	
900	130424071503260417032806	2	NH ₂	NCC1=CC=C(C)C=C1	Holy to	CIC/C(C)=C/(CB@H)(C)C(O)=O	H _M	NOCNC(C)=0		00(01=00=0(00)(0=01)=0	NH,	NC(C@H)(C)C1=CC=CC=C1	HO S	00([0@H](0)0)=0.[5]
800	13042407 13032006 17032804	2	NH ₂		HO TY O		NH ₂				H ₂ N		HO S	
907	1304240/150326081/022803	2	NH ₂	NUC1=CU=C(C)C=C1	₩ ¹	Cic/c(c)=c/(c)@@H)(c)c(0)=0	C NH2	NCCOCHICCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC		00(01=030(00)=N1)=0	HM ~ 101		HO ^Î	
000	150424071503280917092803	2	NH ₂	NGC1=GC=G(C)C=C1	HO TYC	니다(다)=니(U@@H](C)C(O)=O	NAN TOT	1400 1=00(F)=00(0(F)(F)F)=01	o= OH	CUCU=COC(CCU)=N1)≡O	H,N R	nio@njio/01=00=00=01.[R]	HO O S	соцоенј(с)с)=0.[S]
959	130424071504260817022803	2	NH ₂	NUC1=CC=C(C)C=C1	[™] r≁~∘	GIG(C)=G/(C@@H)(C)C(O)=O	Real Provide Address of the second se	NUCERHI(C)C1=CC=CC=C1	o= OH	00(C1=CSC(CCI)=N1)=0	HAI YO	NUCCN1C=CN=C1	- ¹ 0^-	CICC1=CC(C(0)=0)=CC=
2004	1304240/1504260817022810	2	NH ₂	NUC1=CC=C(C)C=C1	HO TO	00000-07222	Real Provide Action of the second sec	мучеренис)C1=CC=CC=C1	OF OH	00(01-005/227) 11-0	RUN CO	NUCUT=UC=C(OC)C(OC)=C1	но	000000000000000000000000000000000000000
961	130424071504260817042805	2		NUC1=CC=C(C)C=C1		UUVC(C)=C/[C@@H](C)C(O)=O		N[U&@H](C)C1=CC=CC=C1	o≓ OH	uc(c1=CSC(CCI)=N1)=0	H,N	NUC1COC(C=CC=C2)=C2O1	HO. O Br R	UC([C@H](C)Br)=0.[R]

observation	full.mol.code2	copies	Amines(X1)	Amines(X1)-smiles	Acid(X1)	Acid(X1)-smiles	Amines(X2)	Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair	Pair3.Acids
962	1304240/150925011/042803	2	NH ₂	NUC1=CU=C(C)C=C1	Holy Co	GC/C(C)=C/(CØ@H)(C)C(C)=C	in the	NGC1=CC=CC(C(F)(F)F)=C1	HO Y Y Y Y	CIC/C(C)=C/[C@@H](C)C(O)=C	HN	NGGUNTGEONEGT	HO O Br R	OC[[O@H](C)BI)=O.[K]
963	130424071509260417042809	2	NH ₂	NCC1=CC=C(C)C=C1	•• ` \$	CIC/C(C)=C/(C@@H)(C)C(O)=O	HUNT	NCC1=CC=CC(C(F)(F)F)=C1	······································	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N	NCC1CCOCC1	HO O Br R	0C([C@H](C)Br)=0.[R]
964	130424071510260317102802	2	NH ₂	NCC1=CC=C(C)C=C1	HO I TO	C[C/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	HO I I I I I I I I I I I I I I I I I I I	CIC/C(C)=C/[C@@H](C)C(O)=O	H _J N S	N(C@@H)(C)C1=CC=CC=C1.[S		CICC1=CC(C(0)=0)=CC=
965	130424081501260217032803	2		N1CONCCC1	₩ ² ¶~~	CIC/C(C)=C/(C@@H)(C)C(O)=O	***	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	"" "	NCCON1C=CN=C1	HO O S	CC([C@H](C)CI)=O.[S]
966	130424081501260317032802	2		N1CONCCC1	HO TATA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
967	130424081501260417032805	2		N1CONCCC1	"	CIC/C(C)=C/(C@@H)(C)C(O)=O	H_N N	NCCNC(C)=O	°↓ CH	OC(C1=CC=C(CCI)C=C1)=O	H _A N AU Y	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=O.[S]
968	130424081501260717032804	2	HN	N1CONCCC1	HO TO	CIC/C(C)=C/[C@@H](C)C(O)=O	L.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)CI)=O.[S]
969	130424081501260717042803	2	HN	N1CONCCC1		CIC/C(C)=C/(C@@H)(C)C(O)=O	A CALINH,	NCC1=CC=C(N(C)C)C=C1	o= ↓ ∩H	OC(C1=CSC(CCI)=N1)=O	HA CA	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
970	130424081501260917022803	2		N1CONCCC1	Horizon	CIC/C(C)=C/[C@@H](C)C(O)=O	nu y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(OCI)=N1)=O	***~~Di	NCCCN1C=CN=C1	HO	CICC1=CC(C(O)=O)=CC=
971	130424081502260717102804	2	HN	N1CONCCC1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	A CANH,	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(OCI)=N1)=0	H ₂ N	N(C@@H)(C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
972	130424081503260317012803	2	HN	N1CONCCC1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HM~~~\D1	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
973	130424081503260317032802	2	HN	N1CONCCC1	no la presidente da	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H _z N	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
974	130424081503261017012803	2	HN	N1CONCCC1	HO LING	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N^	NCC1=CC=C(CI)C=C1	H0 1 1 1	CIC/C(C)=C/(C@@H)(C)C(O)=O	""~~D"	NCCCN1C=CN=C1	Q= OH	OC(C1=CSC(CCI)=N1)=O
975	130424081504260617042803	2	HN	N1CONCCC1	"	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	HM~~~104	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
976	130424081504260617092804	2		N1CONCCC1		CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ₄ R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
977	130424081504261017032808	2	HN	N1CONCCC1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN	NCC1=CC=C(CI)C=C1	₩ ¹ ₩	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N Br	BrC1=CC=C(CN)C=C1	HO S	OC([C@H](C)CI)=O.[S]
978	130424081509260417042803	2	HN	N1CONCCC1		CIC/C(C)=C/[C@@H](C)C(O)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	HO I TAY O	CIC/C(C)=C/[C@@H](C)C(O)=O	100 Mar	NCCCN1C=CN=C1	HO O Br R	OC([C@H](C)Br)=O.[R]
979	130424081510260317022803	2	HN	N1CONCCC1	··· Land	CIC/C(C)=C/[C@@H](C)C(O)=O		CC(C)CCN	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O	HM~~YOI	NCCCN1C=CN=C1		CICC1=CC(C(O)=O)=CC=
980	130424091501260717032802	2	ни	NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	-h	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=0.[S]
981	130424091501260917032801	2	ни	NCCCN1C=CN=C1	₩ ^L tria	CIC/C(C)=C/[C@@H](C)C(O)=O	with	NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	H _M N	NCCC1=CNC2=OC=CC=C21	HO S	OC([C@H](C)Cl)=O.[S]
982	130424091501261017022805	2	ни	NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	HANCO	NCC1=CC=C(CI)C=C1	m to the second	CIC/C(C)=C/(C@@H)(C)C(O)=O	H _A N	NCC1COC(C=CC=C2)=C2O1	HO	CICC1=CC(C(0)=0)=CC=
983	130424091502260317042803	2	ник	NCCCN1C=CN=C1	HO ^L Y ^A	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	~~~ <u>~</u>	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
984	130424091502260417032810	2	ни	NCCCN1C=CN=C1	no la propositiona	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N~H~O	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	HIN COLOR	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)CI)=O.[S]
985	130424091502260517032810	2	н,п	NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCC(C)(C)O	€ CH	OC(C1=CC=C(CCI)C=C1)=O	KIN CO	NCCC1=CC=C(OC)C(OC)=C1	HO S	OC([C@H](C)Cl)=0.[S]
986	130424091502260717032802	2	н,п	NCCCN1C=CN=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	Å.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
987	130424091503260117102804	2	ним	NCCCN1C=CN=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCCOC	orton CI	OC(C1=COC(CCI)=N1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1
988	130424091503260217022804	2	н,п	NCCCN1C=CN=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	HAN DO	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HOLOCO	CICC1=CC(C(O)=O)=CC=
989	130424091503260617092804	2	н,н	NCCCN1C=CN=C1	HO TOTA	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
990	130424091503260917022803	2	нл	NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	NA CONTRACT	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	ни~~р	NCCCN1C=CN=C1	HOLOCA	CICC1=CC(C(0)=0)=CC=
991	130424091503261017012806	2	ни	NCCCN1C=CN=C1	HO Land	CIC/C(C)=C/[C@@H](C)C(0)=O	H _M M^CC	NCC1=CC=C(CI)C=C1	Holy Co	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	CI CI	OC(C1=CSC(CCI)=N1)=O
992	130424091503261017042803	2	н,№~~пп	NCCCN1C=CN=C1	"	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN	NCC1=CC=C(CI)C=C1	┉ᢪ┰ᢩᡧᢇᢩ	CIC/C(C)=C/[C@@H](C)C(O)=O	ни~~	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
993	130424091504260517092804	2	нистр	NCCCN1C=CN=C1	··· Land	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N /	NCC(C)(C)O	€ CH	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]	~О	CCC(O)=O
994	130424091504260817042803	2	H _A N	NCCCN1C=CN=C1		CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	101 - Ch	NCCCN1C=CN=C1	HO. O Br R	OC([C@H](C)Br)=O.[R]

995	130424091504261017012809	2		Amines(X1)-smiles NCCCN1C=CN=C1	Add(XI)	Acid(X1)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	Amines(X2)-smiles NOC1=CC=C(CI)C=C1	Acid(X2)	Acid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O		Amines(X3)-smiles NOC1CCOCC1	Structure of Pair	Pair3.Acids OC(C1=CSC(CCI)=N1)=O
996	130424091509260317012805	2		NCCCN1C=CN=C1	• 1 1 0	СІС/С(С)=С/[С@@H](С)С(О)=О		NOC1=CC=CC(C(F)(F)F)=C1	~ 1 T °	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N Y	NCC1COC(C=CC=C2)=C2O1	о= он	OC(C1=CSC(CCI)=N1)=O
997	130424091510260217012806	2	HAR ~ HEA	NCCCN1C=CN=C1	IN THE C	CIC/C(C)=C/[C@@H](C)C(O)=O	HUN	CC(C)CCN	"	CIC/C(C)=C/[C@@H](C)C(O)=O	\sim	NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
	100 10 100 15 100 00 117 100 00 1	0	H ₂ N ^N NNNN	10000110 011 01	m from	00000 000000000		00/01001/	Hora Contraction		NH ₂		о- Сн	0.0001.0000.01
998	130424091510260417102804	2	H ^I N ~~~ N ~N	NCCCN1C=CN=C1		CIC/C(C)=C/(C(B(BH)(C)C(C)=C		UU(C)UUN	HO I TO	CICIC(C)=CI(OB(@H)(C)C(O)=O	H ₂ N	NCOBOHICICI=CC=CC=C1.[S	0 OH	0=0(0)01=0(0)00=01
999	130424101501260317032802	2	HN	C1CNCCN1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)Cl)=O.[S]
1000	130424101501260517022807	2	HN	C1CNCCN1	HO LANG	CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NCC1=CC(OC)=CC(OC)=C1	HO	CICC1=CC(C(O)=O)=CC=
1001	130424101501260517032802	2	HN	C1CNCCN1	Holgeira	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
1002	130424101501260517102804	2	HN	C1CNCCN1	Holy of a	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N(C@@H)(C)C1=CC=CC=C1.[S	o H	O=C(O)C1=C(C)OC=C1
1003	130424101501260617012809	2		C1CNCCN1	HOLAN	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0		NCC1CCOCC1	Jan a	OC(C1=CSC(CCI)=N1)=O
1004	130424101501260617042803	2		C1CNCCN1	Holy Stra	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	HAN 104	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
1005	130424101501260617042808	2		C1CNCCN1	Lynger and	CIC/C(C)=C/[C@@H](C)C(0)=O	NH ₂	NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H,M^	BrC1=CC=C(CN)C=C1	HO O R	OC([C@H](C)Br)=O.[R]
1006	130424101501260817032802	2		C1CNCCN1	He Lynger	CIC/C(C)=C/[C@@H](C)C(0)=O	$\hat{\mathbf{Q}}$	N[C@@H](C)C1=CC=CC=C1	de	OC(C1=CSC(CCI)=N1)=O	H ₃ N OH	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
1007	130424101502260217012803	2		C1CNCCN1	Holy of a	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN COL	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	···^^_;	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1008	130424101502260317012804	2		C1CNCCN1	Holy of a	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	NCC1=CC=CS1	он ула	OC(C1=COC(CCI)=N1)=O	H ₂ N 0	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
1009	130424101502260517032801	2		C1CNCCN1	Holy in	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O	он С	OC(C1=CC=C(CCI)C=C1)=0	8	NCCC1=CNC2=CC=CC=C21		OC([C@H](C)Cl)=0.[S]
1010	130424101502260717022802	2		C1CNCCN1	Holy of a	CIC/C(C)=C/[C@@H](C)C(O)=O	<u></u>	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NCCO		CICC1=CC(C(O)=O)=CC=
1011	130424101502260717022803	2		C1CNCCN1	Holy Stra	CIC/C(C)=C/[C@@H](C)C(O)=O	4	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NCCCN1C=CN=C1	~ **	CICC1=CC(C(O)=O)=CC=
1012	130424101502260817102804	2		C1CNCCN1	HU LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	\bigcirc	N[C@@H](C)C1=CC=CC=C1	OF OH	OC(C1=CSC(CCI)=N1)=O	HyN	N[C@@H](C)C1=CC=CC=C1.[S	OH CH	0=C(0)C1=C(C)0C=C1
1013	130424101502260917032806	2		C1CNCCN1	- 1 -	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN Y	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	\bigcirc	NC[C@H](C)C1=CC=CC=C1	HO C S	OC([C@H](C)Cl)=0.[S]
1014	130424101502261017012803	2		C1CNCCN1	i j j a	CIC/C(C)=C/[C@@H](C)C(O)=O	Y +,**^{1	NCC1=CC=C(CI)C=C1	остон	CIC/C(C)=C/[C@@H](C)C(O)=O	NH2	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1015	130424101503260417032807	2		C1CNCCN1	lusia	CIC/C(C)=C/[C@@H](C)C(O)=O		NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	~~~~ ^{N1}	NCC1=CC(OC)=CC(OC)=C1	ощон но он	OC([C@H](C)Cl)=0.[S]
1016	130424101503260517012806	2		C1CNCCN1	NO Y Y Y	CIC/C(C)=C/[C@@H](C)C(O)=O	OH OH	NCC(C)(C)O		0C(C1=CC=C(CCI)C=C1)=0	$\langle \rangle$	NC[C@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O
1017	130424101503260917032802	2		C1CNCCN1	™ ¥ ¥ *	CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC(F)=OC(C(F)(F)F)=C1	J. ~	OC(C1=CSC(CCI)=N1)=O	NH ₂	NCCO	о= (он ноо	OC([C@H](C)Cl)=0.[S]
1018	130424101503260917092804	2		C1CNCCN1	in the second se	CIC/C(C)=C/[C@@H](C)C(O)=O	HUMAN'T	NOC1=OC(F)=OC(C(F)(F)F)=C1	о= он	OC(C1=CSC(CCI)=N1)=O	H ₂ N ⁻	N[C@H](C)C1=CC=CC=C1.[R]	×. `	CCC(O)=0
1019	130424101503260917102804	2		C1CNCCN1	HO TATA	CIC/C(C)=C/[C@@H](C)C(0)=O	· · ·	NOC1=CC(F)=CC(C(F)(F)F)=C1	о-{ _{он}	OC(C1=CSC(CCI)=N1)=O	H ₂ N-Y	N[C@@H](C)C1=CC=CC=C1.[S	он N ^{ОН}	O=C(O)C1=C(C)OC=C1
1020	130424101504260217032803	2	NH	C1CNCCN1		CIC/C(C)=C/[C@@H](C)C(O)=O	γ, ····	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCi)=N1)=O	0 ^s	NCCCN1C=GN=C1	HO. 20	OC([C@H](C)Cl)=0.[S]
1021	130424101504260517032802	2		C1CNCCN1	Ho I good a	CIC/C(C)=C/[C@@H](C)C(O)=O		NCC(C)(C)O	OF OH	OC(C1=CC=C(CCI)C=C1)=O	HN NO	NCCO	s s	OC([C@H](C)CI)=0.[S]
1022	12042410160420017022802	2	HN	CICNCON	HO I TO		H ₂ N /		OH CI	00/04=020/001\=N14\=0	H ₂ N		HO O S	CICC1=CC/C/Q)=Q)=CC=
1022	130424101304200917022803	2	HNNNH	CICNCONT	HO I TO	GGGG-GTGBBHJC/C(0)=0	HUN THE	NUC 1=UC(F)=UC(G(F)(F)F)=U1	OH CI	00(01=030(00)=N1)=0	HAN NON	NCCONTC=CN=CT	HO	0001=00(0(0)=0)=00=
1023	130424101509260117022804	2		C1CNCCN1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	w	NCC1=CC=CC(C(F)(F)F)=C1	HO I TO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	но	CICC1=CC(C(O)=O)=CC=
1024	130424101509260117092804	2	HN	C1CNCCN1	Ho I porto	CIC/C(C)=C/[C@@H](C)C(0)=O	HAN CON	NCC1=CC=CC(C(F)(F)F)=C1	Holy Ca	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
1025	130424101509260217012804	2	HN	C1CNCCN1	₩ ⁻¹ ₩~~~	CIC/C(C)=C/[C@@H](C)C(O)=O	wook	NOC1=CC=CC(C(F)(F)F)=C1	₩ ¹ ₩4~0	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₃ N 0	NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
1026	130424101509260217012808	2	HN	C1CNCCN1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	NA CAR	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N C	BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCI)=N1)=O
1027	130424101509260317092801	2	HIN	C1CNCCN1	Holy of a	CIC/C(C)=C/[C@@H](C)C(O)=O	in	NCC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]		OC(C1=CSC(CCI)=N1)=O

observation 1028	full.mol.code2 130424101510260217022803	2		Amines(X1)-smiles C1CNCCN1		Acid(X1)-smiles CIC/C(C)=C/[C@@H](C)C(O)=C	Amines(X2)	Amines(X2)-smiles CC(C)CCN		Acid(X2)-smiles CIC/C(C)=C/[C@@H](C)C(O)=O		Amines(X3)-smiles NCCCN1C=CN=C1	HO CI	Pair3.Acids CICC1=CC(C(O)=O)=CC=
1029	130424101510260417102802	2		C1CNCCN1	Lesso	CIC/C(C)=C/[C@@H](C)C(O)=C		CC(C)CCN		CIC/C(C)=C/[C@@H](C)C(O)=O	HJN	N[C@@H](C)C1=CC=CC=C1.[S		CICC1=CC(C(O)=O)=CC=
1030	130924011502260217102804	2		NCCC1CCOCC1		OC(C1=COC(CCI)=N1)=O	HAN COLO	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N ₄ s	N[C@@H](C)C1=CC=CC=C1.[S	OH	O=C(O)C1=C(C)OC=C1
1031	130924011503260417032804	2		NCCC1CCOCC1	O= (OH ∫C	OC(C1=COC(CCI)=N1)=O	d'	NCCNC(C)=0	≪ √ √	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N~7-0	NCC1=CC=CO1		OC([C@H](C)Cl)=O.[S]
1032	130924011504260517092802	2		NCCC1CCOCC1	O=(OH	OC(C1=COC(CCI)=N1)=O	OH HIN	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]		CICC1=CC(C(O)=O)=CC=
1033	130924011509260217092802	2		NCCC1CCDCC1	o=(oH ∫_N	OC(C1=COC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	bu lance	CIC/C(C)=C/(C@@H)(C)C(O)=O	H,N K R	N(C@H)(C)C1=CC=CC=C1.[R]	ل سلم	CICC1=CC(C(O)=O)=CC=
1034	130924021501260417042806	2		NCCC1CCOCC1	o≓(oH	CICC1=CC(C(O)=O)=CC=C1	HANNING P	NOCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	\bigcirc	NC[C@H](C)C1=CC=OC=C1	HO C R	OC([C@H](C)Br)=O.[R]
1035	130924021501260617092801	2		NCCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	H ₂ NH ₂	N[C@H](C)C1=CC=CC=C1.[R]	Br Shar	OC(C1=CSC(CCI)=N1)=O
1036	130924021502260817032806	2		NCCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1	\bigcirc	N[C@@H](C)C1=CC=CC=C1	6H N	OC(C1=CSC(CCI)=N1)=O	\bigcirc	NC[C@H](C)C1=CC=CC=C1		OC([C@H](C)CI)=O.[S]
1037	130924021503260817102803	2		NCCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1		N[C@@H](C)C1=CC=CC=C1	o≓(_{OH}	OC(C1=CSC(CCI)=N1)=O	H ₂ NH2	N[C@@H](C)C1=CC=CC=C1.[S		OC([C@H](C)CI)=O.[S]
1038	130924021503260917092802	2		NCCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1	H,NYYYY	NOC1=CC(F)=CC(C(F)(F)F)=C1	остон Сула	OC(C1=CSC(CCI)=N1)=O	H,N	N[C@H](C)C1=CC=CC=C1.[R]		CICC1=CC(C(O)=O)=CC=
1039	130924021504260617032809	2		NCCC1CCOCC1	in the second se	CICC1=CC(C(O)=O)=CC=C1		NOC1=CC=CC=C1	от _{он}	OC(C1=CC=C(CCI)C=C1)=0		NCC1CCOCC1	HO O S	OC([C@H](C)CI)=O.[S]
1040	130924021504260617102804	2		NCCC1CCOCC1	- C	CICC1=CC(C(O)=O)=CC=C1		NOC1=CC=CC=C1	бн Ф	OC(C1=CC=C(CCI)C=C1)=0	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S		O=C(O)C1=C(C)OC=C1
1041	130924021504261017102804	2		NCCC1CCOCC1		CICC1=CC(C(O)=O)=CC=C1	~ ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~	NOC1=CC=C(CI)C=C1	du Holigani co	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
1042	130924021509260117102804	2		NCCC1CCOCC1	, in the second	CICC1=CC(C(O)=O)=CC=C1	HAN Y Y	NOC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H,N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
1043	130924021509260417022806	2		NCCC1CCOCC1	in the second se	CICC1=CC(C(O)=O)=CC=C1	HAR Y Y	NOC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	\bigcirc	NC[C@H](C)C1=CC=CC=C1		CICC1=CC(C(O)=O)=CC=
1044	130924031501260417042804	2		NCCC1CCOCC1	j m	OC(C1=CSC(CCI)=N1)=O	HAN N PO	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O		NCC1=CC=CO1	HO O R	OC([C@H](C)Br)=O.[R]
1045	130924031501260517102802	2		NCCC1CCOCC1	о= _{он}	OC(C1=CSC(CCI)=N1)=O	OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ₄ s	N[C@@H](C)C1=CC=CC=C1.[S	Br	CICC1=CC(C(O)=O)=CC=
1046	130924031501260617032801	2		NCCC1CCOCC1	о= с _{он}	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	R	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)CI)=O.[S]
1047	130924031501260617042804	2		NCCC1CCOCC1	O=OH	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1	bн o	OC(C1=CC=C(CCI)C=C1)=O		NCC1=CC=CO1	HO C R	OC([C@H](C)Br)=O.[R]
1048	130924031501260717032807	2		NCCC1CCOCC1	OH SAN	OC(C1=CSC(CCI)=N1)=O	× 10.	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O		NCC1=CC(OC)=CC(OC)=C1	HO O S	OC([C@H](C)CI)=O.[S]
1049	130924031501260717092803	2		NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	- - 10 -	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N	N[C@H](C)C1=CC=CC=C1.[R]		OC([C@H](C)CI)=O.[S]
1050	130924031501260717092804	2		NCCC1CCOCC1	OH SAN CI	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N(C@H)(C)C1=CC=CC=C1.[R]		CCC(O)=O
1051	130924031502260217012804	2		NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O	" " Cly	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O		NCC1=CC=CO1		OC(C1=CSC(CCI)=N1)=O
1052	130924031502260417022804	2		NCCC1CCOCC1	он 	OC(C1=CSC(CCI)=N1)=O	H _A N~ ^H + ^o	NCCNC(C)=0	OH	CC(C1=CC=C(CCI)C=C1)=O	H ₂ N 0	NCC1=CC=CO1	но	CICC1=CC(C(O)=O)=CC=
1053	130924031502260517032802	2		NCCC1CCOCC1	он Сула	OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O		NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
1054	130924031502260817012803	2		NCCC1CCOCC1	OH Jana	OC(C1=CSC(CCI)=N1)=O	Ŷ	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	······································	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1055	130924031502261017012808	2		NCCC1CCOCC1		OC(C1=CSC(CCI)=N1)=O		NOC1=CC=C(CI)C=C1	HOLY C	CIC/C(C)=C/[C@@H](C)C(O)=O	H _A N^	BrC1=CC=C(CN)C=C1		OC(C1=CSC(CCI)=N1)=O
1056	130924031502261017032801	2		NCCC1CCOCC1	OH Jan Ci	OC(C1=CSC(CCI)=N1)=O	H _A M ^A CA _a	NCC1=CC=C(CI)C=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	8.	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=O.[S]
1057	130924031502261017092804	2	HAN	NCCC1CCOCC1	OH	OC(C1=CSC(CGI)=N1)=O	H,M^CC	NCC1=CC=C(CI)C=C1	Holyng a	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]		CCC(0)=0
1058	130924031503260317032802	2	HAN CO	NCCC1CCOCC1	OH	OC(C1=CSC(CCI)=N1)=O	H _J N S	NCC1=CC=CS1	J. Carlo	OC(C1=COC(CCI)=N1)=O	H ₂ N ~- OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
1059	130924031503260317032805	2	HAN	NCCC1CCOCC1	OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N S	NCC1=CC=CS1	OH	OC(C1=COC(CCI)=N1)=O	H_N	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)Cl)=O.[S]
1060	130924031503260317102804	2	H ₂ N~	NCCC1CCOCC1	OH OH OH OH	OC(C1=CSC(CCi)=N1)=O	H ₂ N	NCC1=CC=CS1	он	OC(C1=COC(CCI)=N1)=O	H,N S	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	0=C(0)C1=C(C)0C=C1

1061	130924031503260617102802	2	H ₂ N	NCCC1CCCCC1	OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N[C@@H](C)C1=CC=CC=C1.[S	но	CICC1=CC(C(0)=0)=CC=
1062	130924031503260817092804	2	H ₂ N		OC(C1=CSC(CCI)=N1)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	HJN K	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
1063	130924031504260317022803	2	H ₂ N		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	HAI~~101	NCCCN1C=CN=C1	но	CICC1=CC(C(O)=O)=CC=
1064	130924031504260317092803	2	H ₂ N		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H _J N	N[C@H](C)C1=CC=CC=C1.[R]	HO O S	OC([C@H](C)Cl)=O.[S]
1065	130924031504260517032803	2	H ₂ N		OC(C1=CSC(CCI)=N1)=O		NCC(C)(C)O		OC(C1=CC=C(CCI)C=C1)=O	······································	NCCCN1C=CN=C1	HO S	OC([C@H](C)Cl)=O.[S]
1066	130924031509260117012803	2	H ₂ N		OC(C1=CSC(CCl)=N1)=O		NOC1=CC=CC(C(F)(F)F)=C1	m land	CIC/C(C)=C/[C@@H](C)C(O)=O	HM ~ M)H	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1067	130924031509260217012803	2	H ₂ N		OC(C1=CSC(CCI)=N1)=O		NOC1=CC=CC(C(F)(F)F)=C1	m land	CIC/C(C)=C/[C@@H](C)C(O)=O	ни Оч	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1068	130924031509260217032804	2	H ₂ N		OC(C1=CSC(CCI)=N1)=O		NCC1=CC=CC(C(F)(F)F)=C1	HO I TAY O	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)CI)=O.[S]
1069	130924031510260317012803	2	H ₂ N		OC(C1=CSC(CCl)=N1)=O		CC(C)CCN	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HM	NCCCN1C=CN=C1	CI CI CI	OC(C1=CSC(CCI)=N1)=O
1070	130924041501260817102804	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=0	H ₂ N	N[O@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
1071	130924041501260917012803	2	H ₂ N-~~		CIC/C(C)=C/(C@@H)(C)C(O)=O	w p X'	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HAL-10	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1072	130924041501260917032808	2	H ₂ N	NCCC1CCOCC1	CIC/C(C)=C/(C@@H)(C)C(O)=O		NOC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=0	H,N Br	BrC1=CC=C(CN)C=C1	HO O S	OC([C@H](C)Cl)=O.[S]
1073	130924041501261017102802	2	H ₂ N		CIC/C(C)=C/(C@@H)(C)C(O)=O	H,M^CC	NCC1=CC=C(CI)C=C1	HO I TAL	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	но	CICC1=CC(C(O)=O)=CC=
1074	130924041502260217092804	2	H ₂ N		CIC/C(C)=C/(C@@H)(C)C(O)=O		NCC1=CC=C(S(=0)(C)=0)C=C	OF OH	OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(0)=0
1075	130924041502260317032809	2	H ₂ N		CIC/C(C)=C/(C@@H)(C)C(O)=O	H ₂ N S	NCC1=CC=CS1		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1CCOCC1	s s	OC([C@H](C)Cl)=O.[S]
1076	130924041502260817012808	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(O)=O		N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H _A N Br	BrC1=CC=C(CN)C=C1	order CI	OC(C1=CSC(CCI)=N1)=O
1077	130924041503260217032802	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(0)=0		NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCi)=N1)=O	H ₂ N OH	NCCO	HO S	OC([C@H](C)CI)=O.[S]
1078	130924041503260917042803	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(O)=O		NOC1=CC(F)=OC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	HAI~	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
1079	130924041504260617032801	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(0)=0	NH ₂	NCC1=CC=CC=C1	or the second se	OC(C1=CC=C(CCI)C=C1)=O	HAN	NCCC1=CNC2=CC=CC=C21	HO S	OC([C@H](C)CI)=O.[S]
1080	130924041509260217032802	2	H2N		CIC/C(C)=C/(C@@H)(C)C(O)=O	w A	NOC1=CC=CC(C(F)(F)F)=C1	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)Cl)=O.[S]
1081	130924041509260217032809	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(O)=O	in the	NCC1=CC=CC(C(F)(F)F)=C1	₩ ^{\$}	CIC/C(C)=C/[C@@H](C)C(O)=O	H _M N	NCC1CCOCC1	HO S	OC([C@H](C)Cl)=0.[S]
1082	130924041510260317022806	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(0)=0		CC(C)CCN	HO I TAY O	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[C@H](C)C1=CC=CC=C1	HO I COTO	CICC1=CC(C(O)=O)=CC=
1083	130924041510260317092803	2	H ₂ N		CIC/C(C)=C/(C@@H)(C)C(O)=O		CC(C)CCN	₩ ^Ĺ Ţ ^ĸ Ţ^a	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO S	OC([C@H](C)Cl)=0.[S]
1084	130924041510260417032805	2	H ₂ N		CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	CC(C)CCN	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H,N	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=0.[S]
1085	131024011501260417022809	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	OC(C1=COC(CCI)=N1)=O	H _N N	NOCNC(C)=0	CH CO	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	N0C1CC0CC1	Ho L	CICC1=CC(C(O)=O)=CC=
1086	131024011501261017032803	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	OC(C1=COC(CCI)=N1)=O	H,M^C	N0C1=CC=C(Cl)C=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	ни~~D	NCCCN1C=CN=C1	HO O S	OC([C@H](C)CI)=O.[S]
1087	131024011502260217032802	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	OC(C1=COC(CCI)=N1)=0		NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=0	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
1088	131024011502260417022809	2	H ₂ N	NUUT=CC(F)=C(F)C=C	UC(C1=COC(CCI)=N1)=0	H ₂ N~ ^H Y ^O	NUCNC(C)=0	€ OH	UU(U1=CC=C(CCI)C=C1)=0	H _k N	NUC1CC0CC1		CICC1=CC(C(0)=0)=CC=
1089	131024011502260617012803	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	OC(C1=COC(CCI)=N1)=O	NH ₂	N0C1=CC=CC=C1	° ↓ ↓ ↓ ↓ ↓	OC(C1=CC=C(CCI)C=C1)=O	***~~D*	NCCCN1C=CN=C1	→ → CI	OC(C1=CSC(CCI)=N1)=O
1090	131024011502260717042805	2	H ₂ N	NCC1=CC(F)=C(F)C=C	OC(C1=COC(CCI)=N1)=O	40, m,	NCC1=CC=C(N(C)C)C=C1	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H _J N O	NCC1COC(C=CC=C2)=C2O1	HO O Br R	OC([C@H](C)Br)=O.[R]
1091	131024011503260717032802	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	OC(C1=COC(CCI)=N1)=O	h Quan,	NCC1=CC=C(N(C)C)C=C1	o= OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ~~ OH	NCCO	HO CO S	OC([C@H](C)Cl)=O.[S]
1092	131024011503260717102804	2	H ₂ N	NULL1=CC(F)=C(F)C=C	UC(C1=COC(CCI)=N1)=O	h Quan,	NUC1=CC=C(N(C)C)C=C1	O= OH	00(C1=CSC(CCI)=N1)=0	H ₂ N S	N(U@@H)(C)C1=CC=CC=C1.[S	OH OH	U=C(0)C1=C(C)OC=C1
1093	131024011504260617012803	2	H ₂ N F	NUCT=CC(F)=C(F)C=C	UC(C1=COC(CCI)=N1)=0		NUU1=CC=CC=C1	€ OH	UU(U1=CC=C(CCI)C=C1)=0	HAN YON	NUUCN1C=CN=C1	o=↓ OH	UC(C1=CSC(CCI)=N1)=O

observation 1094	full.mol.code2 131024011504260717032801	2	Amines(X1)	Amines(X1)-smiles NCC1=CC(F)=C(F)C=C		Acid(X1)-smiles OC(C1=COC(CCI)=N1)=O	Amines(X2)	Amines(X2)-smiles NCC1=CC=C(N(C)C)C=C1		Acid(X2)-smiles OC(C1=CSC(CCI)=N1)=O	Amines(X3)	Amines(X3)-smiles NCCC1=CNC2=CC=CC=C21	HO O S	Pair3.Acids OC([C@H](C)Cl)=O.[S]
1095	131024021501260417012803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	но	CICC1=CC(C(O)=O)=CC=C1	H _M N~ ^H + ^O	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=0		NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1096	131024021501260617032802	2	F H ₂ N	NCC1=CC(F)=C(F)C=C	HO TO TO	CICC1=CC(C(O)=O)=CC=C1		NOC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N OH	NCCO	но о	OC([C@H](C)Cl)=O.[S]
1097	131024021501260717032802	2	F H ₂ N	NCC1=CC(F)=C(F)C=C	m ²	CICC1=CC(C(O)=O)=CC=C1	40.00	NOC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=0.[S]
1098	131024021501261017022806	2	F H ₂ N	NCC1=CC(F)=C(F)C=C	HIN TO THE REAL PROPERTY OF	CICC1=CC(C(O)=O)=CC=C1	H ₂ N ¹ Cl	NCC1=CC=C(CI)C=C1	юн	CIC/C(C)=C/[C@@H](C)C(O)=O	\mathbf{Q}	NC[C@H](C)C1=CC=CC=C1	He Land	CICC1=CC(C(O)=O)=CC=
1099	131024021501261017032803	2	F HyN^	NCC1=CC(F)=C(F)C=C	بر سال	CICC1=CC(C(O)=O)=CC=C1	H _J N C	NCC1=CC=C(CI)C=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ NH ₂	NCCCN1C=CN=C1	HU U S	OC([C@H](C)Cl)=0.[S]
1100	131024021502260117032803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	···	CICC1=CC(C(O)=O)=CC=C1	H ₂ N O	NCCOC		OC(C1=COC(CCI)=N1)=O	H.M.~~104	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=O.[S]
1101	131024021502260217032804	2	H ₂ N C	NCC1=CC(F)=C(F)C=C	ностор	CICC1=CC(C(O)=O)=CC=C1	****	NCC1=CC=C(S(=O)(C)=O)C=C		OC(C1=COC(CCI)=N1)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=0.[S]
1102	131024021502260717092803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	HOLOCO	CICC1=CC(C(O)=O)=CC=C1	A Com	NCC1=CC=C(N(C)C)C=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	HO S	0C([C@H](C)Cl)=0.[S]
1103	131024021502261017092804	2	H ₂ N	NCC1=CC(F)=C(F)C=C	HO ^L	CICC1=CC(C(O)=O)=CC=C1	ни	NCC1=CC=C(CI)C=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	N(C@H)(C)C1=CC=CC=C1.[R]	∼гр⁰	CCC(O)=O
1104	131024021503260417102803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	HO CON	CICC1=CC(C(O)=O)=CC=C1	нл~н~	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N ₂ s	N[C@@H](C)C1=CC=CC=C1.[S	HO S	OC([C@H](C)Cl)=0.[S]
1105	131024021503260617022803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	HO ^L LO ^L O	CICC1=CC(C(O)=O)=CC=C1		NCC1=CC=CC=C1	ortication of the second seco	OC(C1=CC=C(CCI)C=C1)=0	HAIL NON	NCCON1C=CN=C1	HOLOCI	CICC1=CC(C(O)=O)=CC=
1106	131024021503260917042803	2	H ₂ N	NCC1=CC(F)=C(F)C=C		CICC1=CC(C(O)=O)=CC=C1	""	NCC1=CC(F)=CC(C(F)(F)F)=C1		OC(C1=CSC(CCI)=N1)=O	···^^p	NCCCN1C=CN=C1	HO O R	OC([C@H](C)Br)=O.[R]
1107	131024021509260117032804	2	H ₂ N	NCC1=CC(F)=C(F)C=C		CICC1=CC(C(O)=O)=CC=C1	1.11	NCC1=CC=CC(C(F)(F)F)=C1	HOLINA	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO S	OC([C@H](C)CI)=O.[S]
1108	131024021509260317012803	2	H _A N C	NCC1=CC(F)=C(F)C=C		CICC1=CC(C(O)=O)=CC=C1	en C	NCC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M ~ M _ M	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1109	131024021509260417012803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	no l	CICC1=CC(C(O)=O)=CC=C1	w	NCC1=CC=CC(C(F)(F)F)=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	HAN NON	NCCCN1C=CN=C1		OC(C1=CSC(CCI)=N1)=O
1110	131024021509260417022803	2	H ₂ N	NCC1=CC(F)=C(F)C=C	Hologra	CICC1=CC(C(O)=O)=CC=C1	nu C	NCC1=CC=CC(C(F)(F)F)=C1		CIC/C(C)=C/[C@@H](C)C(O)=O	1.vr~10v	NCCCN1C=CN=C1	но	CICC1=CC{C(O)=O)=CC=
1112	131024031501260317092804	2	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H ₂ N	NCC1=CC=CS1	CI CH CH	OC(C1=COC(CCI)=N1)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
1113	131024031501260417022809	2	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H _N N	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	но	CICC1=CC(C(O)=O)=CC=
1114	131024031501260417032809	2	H ₂ N	NCC1=CC(F)=C(F)C=C	o=↓ OH	OC(C1=CSC(CCI)=N1)=O	H _N N ^H Y ⁰	NOCNC(C)=O	OH CI	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=O.[S]
1115	131024031501260417102801	2	H ₂ N	NCC1=CC(F)=C(F)C=C	O=OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N~ ^H ¢ ^O	NCCNC(C)=0	ortice OH	0C(C1=CC=C(CCI)C=C1)=0	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S		OC(C1=CSC(CCI)=N1)=O
1116	131024031501260417102804	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	C→ C→ OH	OC(C1=CSC(CCI)=N1)=O	н, л-~^Ц~ °	NCCNC(C)=O		OC(C1=CC=C(CCI)C=C1)=O	H,N	N[C@@H](C)C1=CC=CC=C1.[S	of the second	O=C(O)C1=C(C)OC=C1
1117	131024031501260817022802	2	H ₂ N	NCC1=CC(F)=C(F)C=C	O=OH	OC(C1=CSC(CCI)=N1)=O	Real Provide Action of the second sec	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HOLICIA	CICC1=CC(C(O)=O)=CC=
1118	131024031501261017012803	2	H ₂ N	NCC1=CC(F)=C(F)C=0	OF OH	OC(C1=CSC(CCI)=N1)=O	H _A N C	NCC1=CC=C(CI)C=C1	HO ^L TA	CIC/C(C)=C/[C@@H](C)C(O)=O	H.N.~~NN	NCCON1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
1119	131024031501261017022803	2	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H _A N CO	NCC1=CC=C(CI)C=C1	HO TATA	CIC/C(C)=C/[C@@H](C)C(O)=O	H,M ~ NON	NCCCN1C=CN=C1	Ho ¹ () ()	CICC1=CC(C(O)=O)=CC=
1120	131024031502260417032810	2	H ₂ N F	NCC1=CC(F)=C(F)C=C	OF OH	OC(C1=CSC(CCI)=N1)=O	H _N N	NCCNC(C)=0		0C(C1=CC=C(CCI)C=C1)=0	NUT CO	NCCC1=CC=C(OC)C(OC)=C1	HO O S	0C([C@H](C)CI)=0.[S]
1121	131024031502260517092804	2	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H ₂ N H	NCC(C)(C)O	o tra	OC(C1=CC=C(CCI)C=C1)=0	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	∽О	CCC(O)=O
1122	131024031503260217012803	2	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	"	NCC1=CC=C(S(=0)(C)=0)C=C		OC(C1=COC(CCI)=N1)=O	H,V ~ NOV	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
1123	131024031503260417032801	2	H ₂ N	NCC1=CC(F)=C(F)C=C		OC(C1=CSC(CCI)=N1)=O	H _N N	NCCNC(C)=0	°↓ OH	OC(C1=CC=C(CCI)C=C1)=O	HAN SHA	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=0.[S]
1124	131024031503260517032803	2	Han	NUC1=CC(F)=C(F)C=C	o= € OH	00(C1=03C(CCI)=N1)=0	NH ₂	NUCT=CC=CC=C1	of the second se	UU(U1=UU=C(CCI)C=C1)=0	HAN NON	NUCCNTC=CN=C1	HO O S	UU([U@H](C)CI)=0.[S]
1125	131024031503260617032809	2	H,N T	NCC1=CC(F)=C(F)C=C	o=↓ OH	OC(C1=CSC(CCi)=N1)=O	NH ₂	NOC1=CC=CC=C1		0C(C1=CC=C(CCI)C=C1)=0	H ₂ N	NCC1CCOCC1	HO CI S	0C([C@H](C)Cl)=0.[S]
1126	131024031503260917032808	2	H ₂ N	NUC1=CC(F)=C(F)C=C	O-CH	UU(C1=CSC(CCI)=N1)=O	HUNTON	NUC1=CC(F)=CC(C(F)(F)F)=C1	OF OH	00(C1=CSC(CCI)=N1)=0	H _A N Br	BrU1=CC=C(CN)C=C1	HO O S	uu([C@H](C)Cl)=0.[S]
1127	131024031504260417022809	2	Han	NUC1=CC(F)=C(F)C=C	o= OH	UU(C1=CSC(CCI)=N1)=O	H ₂ N~N	NGCNC(C)=O	of the second se	00(01=CC=C(CCI)C=C1)=0	H ₂ N-	NGC1000001	HOLOCA	CIUC1=CC(C(0)=0)=CC=

observation	full.mol.code2	copies Amines(X1)	Amines(X1)-smiles A	cid(X1) Acid(X1)-smi	les Amines(X2) Amines(X2)-smiles	Acid(X2)	Acid(X2)-smiles	Amines(X3)	Amines(X3)-smiles	Structure of Pair	Pair3.Acids
1120	101024001004200011102004		F		H ₂ N		of the second	00(01-00-0(00))0-01)-0	s s	ntogenitors - co-co-chio		0-0(0)01-0(0)00-01
1129	131024031504260817032802	2 H ₂ N	NCC1=CC(F)=C(F)C=C			N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H ₂ N OH	NCCO	HO O S	OC([C@H](C)CI)=O.[S]
1130	131024031504261017092804	² H ₂ N	F NCC1=CC(F)=C(F)C=C	CI OC(C1=CSC(CCI)=N	H ₂ N	NCC1=CC=C(CI)C=C1	HO	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	ОН	CCC(O)=O
1131	131024031509260317102804	2 H ₂ N	VCC1=CC(F)=C(F)C=C	CI OC(C1=CSC(CCI)=N	ни	NOC1=CC=CC(C(F)(F)F)=C1	HOLING	CIC/C(C)=C/[C@@H](C)C(O)=O	H _J N	N[C@@H](C)C1=CC=CC=C1.[S	OH OH	O=C(O)C1=C(C)OC=C1
1132	131024031509260417022809		F NCC1=CC(F)=C(F)C=C	OH OC(C1=CSC(CCI)=N		VCC1=CC=CC(C(F)(F)F)=C1	HO LING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1CCOCC1	HO ¹ CCC	CICC1=CC(C(O)=O)=CC=
1133	131024031510260317012803		F NCC1=CC(F)=C(F)C=C			CC(C)CCN	HO LING	CIC/C(C)=C/(C@@H)(C)C(O)=O	HAN ~ YOU	NCCCN1C=CN=C1	O=CH	OC(C1=CSC(CCI)=N1)=O
1134	131024031510260317032803	2 H ₂ N	NCC1=CC(F)=C(F)C=C			CC(C)CCN	HO I I I I	CIC/C(C)=C/[C@@H](C)C(O)=O	***~~D*	NCCCN1C=CN=C1	HO O S	OC([C@H](C)Cl)=0.[S]
1135	131024031510260417032804		NCC1=CC(F)=C(F)C=C		1)=0	CC(C)CCN	HOLE	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N	NCC1=CC=CO1	HO O S	OC([C@H](C)Cl)=O.[S]
1136	131024041501260217032805	2 H ₂ N	NCC1=CC(F)=C(F)C=C		(C)C(O)=0	NCC1=CC=C(S(=0)(C)=0)C=0		OC(C1=COC(CCI)=N1)=O	Hand	NCC1COC(C=CC=C2)=C2O1	HO O S	OC([C@H](C)CI)=O.[S]
1137	131024041501260417022806	2 H ₂ N	F NCC1=CC(F)=C(F)C=C		(C)C(O)=0	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=OC=C1	HO ¹ CCC	CICC1=CC(C(O)=O)=CC=
1138	131024041501260417032806	2 H ₂ N	NCC1=CC(F)=C(F)C=C	CIC/C(C)=C/(C@@H)	(C)C(O)=0	NCCNC(C)=0	OH CI	OC(C1=CC=C(CCI)C=C1)=O	NH ₂	NC[C@H](C)C1=CC=OC=C1	HO O S	OC([C@H](C)Cl)=0.[S]
1139	131024041501260417032807		NCC1=CC(F)=C(F)C=C		(C)C(O)=0	NCCNC(C)=0	or the second se	0C(C1=CC=C(CCI)C=C1)=0	· ↓ · · ·	NCC1=CC(OC)=CC(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
1140	131024041501260617032804	2 H ₂ N	NCC1=CC(F)=C(F)C=C		(C)C(O)=0	NCC1=CC=CC=C1		OC(C1=CC=C(CCI)C=C1)=0	II2N 0	NCC1=CC=CO1	HO S	OC([C@H](C)Cl)=O.[S]
1141	131024041501260817032807		NCC1=CC(F)=C(F)C=C		(C)C(O)=O	N[C@@H](C)C1=CC=CC=C1	CH CI	OC(C1=CSC(CCI)=N1)=O		NCC1=CC(OC)=CC(OC)=C1	HO S	OC([C@H](C)Cl)=O.[S]
1142	131024041501260917012803	2 H ₂ N	NCC1=CC(F)=C(F)C=C		(C)C(O)=0	Y NOC1=OC(F)=OC(O(F)(F)F)=O		OC(C1=CSC(CCI)=N1)=O	H.N.~ N_O	NCCCN1C=CN=C1	O= OH	OC(C1=CSC(CCI)=N1)=O
1143	131024041501260917032809	2 H ₂ N	NCC1=CC(F)=C(F)C=C		(C)C(O)=0	X ^F NOC1=OC(F)=OC(O(F)(F)F)=O		OC(C1=CSC(CCI)=N1)=O	H _J N	NCC1CCOCC1	HO O S	OC([C@H](C)Cl)=O.[S]
1144	131024041502260617032808		F NCC1=CC(F)=C(F)C=C		(C)C(O)=0	NCC1=CC=CC=C1	of the second se	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N ¹	BrC1=CC=C(CN)C=C1	HO S	OC([C@H](C)Cl)=O.[S]
1145	131024041502261017092802		F NCC1=CC(F)=C(F)C=C		(C)C(O)=O	NCC1=CC=C(CI)C=C1	HO TO A	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]		CICC1=CC(C(O)=O)=CC=
1146	131024041503260417032801	2 H ₂ N	F HO		(C)C(O)=0	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=O	нл	NCCC1=CNC2=CC=CC=C21	HO O S	OC([C@H](C)Cl)=0.[S]
1147	131024041504260417032804	2 H ₂ N	F NCC1=CC(F)=C(F)C=C		(C)C(O)=O	NCCNC(C)=0 ≠0	o transformation of the second	OC(C1=CC=C(CCI)C=C1)=O	H ₂ N O	NCC1=CC=CO1	HO O S	СС([C@H](C)Cl)=0.[S]
1148	131024041504260417092804		NCC1=CC(F)=C(F)C=C		(C)C(O)=O	NCCNC(C)=0		OC(C1=CC=C(CCI)C=C1)=0	H ₂ N R	N[C@H](C)C1=CC=CC=C1.[R]	Он	CCC(O)=O
1149	131024041504260717032802		NCC1=CC(F)=C(F)C=C		(C)C(O)=0	NCC1=CC=C(N(C)C)C=C1	o= ↓ −N OH	OC(C1=CSC(CCI)=N1)=O	H ₂ N ^{OH}	NCCO	HO O S	OC([C@H](C)Cl)=0.[S]
1150	131024041504260817032805		PF	CIC/C(C)=C/(C@@H)	(C)C(O)=O	N[C@@H](C)C1=CC=CC=C1		OC(C1=CSC(CCI)=N1)=O	H _L N ^A U ^O	NCC1COC(C=CC=C2)=C2O1	HO S	OC([C@H](C)Cl)=0.[S]
1151	131024041509260317032803		NCC1=CC(F)=C(F)C=C		(C)C(O)=0	X ¹	HO LANG	CIC/C(C)=C/[C@@H](C)C(O)=O	HAI YO	NCCCN1C=CN=C1	HO S	OC([C@H](C)CI)=O.[S]
1152	131024041509260317102804		NCC1=CC(F)=C(F)C=C		(C)C(O)=0	X ^F	HO LING	CIC/C(C)=C/[C@@H](C)C(O)=O	H ₂ N S	N[C@@H](C)C1=CC=CC=C1.[S	OH O	0=C(0)C1=C(C)0C=C1
1153	131024041509260417022806		NCC1=CC(F)=C(F)C=C		(C)C(O)=O	NCC1=CC=CC(C(F)(F)F)=C1	но	CIC/C(C)=C/[C@@H](C)C(O)=O	NH ₂	NC[C@H](C)C1=CC=OC=C1	HO	CICC1=CC(C(O)=O)=CC=
Section 11: Analysis of ring-closure via the Michael (thiol-enone) reaction

Linear analogs of DDD and DDA were synthesized with acrylic acid at the X3 position on 10 & 160 μ M beads following general SPS method. Compound DDD and DDA have complete cyclization after 8hrs. Thiol protecting STMP group was removed from the linear precursor and it was suspended in 2x PBST buffer at 37°C for 12 hrs. DMSO solution of BnBr was added to beads suspended in PBST buffer (final conc, 1.0M, 150uL) and incubated for an hour at 37°C. Similarly, 10 μ M beads were treated with DMSO solution of mBBr dye (final conc, 1mM, 150ul, PBS). After thiol alkylations, they were washed, 160 μ M beads were TFA cleaved and analyzed over LCMS. 10 μ M beads were suspended in PBST buffer, transferred to BD FACS tube and their fluorescence was measured.

Incomplete cyclization was observed for both DDD and DDA analogs for thiol-ene based ring closure.

Analysis of ring-closure via flow-cytometry:



Cyclization of DDA-analog:

Incomplete cyclization was observed on 160 μ M beads but 10 μ M beads seems to have completed cyclization. Ring closure via thiol-ene reaction appears to be slower compared to halide displacement based reaction.









Cyclization of DDD analog:

Incomplete cyclization was observed on 160 μ M beads but 10 μ M beads seems to have completed cyclization. Ring closure via thiol-ene reaction appears to be slower compared to halide displacement based reaction.







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