

Supplementary Material

Prediction of the classification, labelling and packaging Regulation H-statements with confidence using Conformal Prediction with N-grams and Molecular Fingerprints

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Table S1. H-statement groups and included H-statements and number compounds in each class.

H-statement group	Included H-statements	Corresponding endpoints	#cmpds H-statement class	#cmpds non-H-statement class
H30x012345	H300, H301, H302, H303, H304. H305	Fatal or harmful if swallowed	4481	3108
H31x0123	H310, H311, H312, H313	Fatal or harmful in contact with skin	1067	5942
H31x57	H315, H317	Skin irritation	4931	5342
H33x0123	H330, H331, H332, H333	Fatal or harmful if inhaled	393	8433
H33x45	H334, H335	Respiratory irritation	1708	1994
H34x	All subcategories of H34	Genetic toxicity	393	8433
H35x	All subcategories of H35	Carcinogenicity	510	2769
H36x01	H360x,H361x	May damage fertility or unborn child	902	4894
H40x	All subcategories of H40	Toxic to aquatic life	1754	7615
H41x	All subcategories of H41	Toxic to aquatic life with long lasting effects	4847	5040

Pseudo code for retrieving H-statements

1. IMPORT python libraries BeautifulSoup and pandas
2. Initialize an empty pandas DataFrame: df
 - 2.1 id_list = ["Display Name", "EC Number", "EC Name", "CAS Number", "Molecular formula", "IUPAC Name"]
 - 2.2 type_list = ["Composition", "Origin"]
 - 2.2 admin_list = ["Total range", "Registered as", "Submitted"]
 - 2.3 human_health_classes = ["Acute toxicity - oral", "Acute toxicity - dermal", "Acute toxicity - inhalation", "Skin corrosion / irritation", "Serious eye damage / eye irritation", "Respiratory sensitisation", "Skin sensitisation", "Aspiration hazard", "Reproductive toxicity", "Effects on or via lactation", "Germ cell mutagenicity", "Carcinogenicity", "1. Specific target organ toxicity - single (STOT-SE)", "1. Specific target organ toxicity - repeated (STOT-RE)"]
 - 2.4 ecotox_classes = ["Hazardous to the aquatic environment (acute / short-term)", "Hazardous to the aquatic environment (long-term)", "Hazardous to the ozone layer"]
 - 2.5 columns of df = "id"+id_list+type_list+admin_list+human_health_list+ecotox_list
3. Define the function "fetch_data_for_id(i)" to fetch data for a given id i
 - 3.1 Create a row in the DataFrame for the current id: df[i, "id"] = i
 - 3.2 Initialize the URLs for i
 - 3.2.1 url0 = "https://echa.europa.eu/registration-dossier/-/registered-dossier/i/1/1"
 - 3.2.2 url1 = "https://echa.europa.eu/registration-dossier/-/registered-dossier/i/1/2"
 - 3.2.3 url2 = "https://echa.europa.eu/registration-dossier/-/registered-dossier/i/2/1"
 - 3.3 Make requests to the URLs and parse the HTML content to get information into df with BeautifulSoup:
 - 3.3.1 columns in id_list can be fetched from url0 under <h3> title "sIdentification"
 - 3.3.2 columns in type_list can be fetched from url0 under <h3> title "sTypeOfSubstance"
 - 3.3.3 columns in admin_list can be fetched from url1 in a <div> object with id "SectionContent"
 - 3.3.4 columns in human_health_classes can be fetched from url2 in a <div> object with id "collapseHealthHazards1CollapseGroup1"
 - 3.3.5 columns in ecotox_classes can be fetched from url2 in a <div> object with id "collapseEnvironmentalHazards1CollapseGroup1"

Example (get df.loc[i, "Display Name"]):

```

html_list = list of all html objects in url0 fetched by BeautifulSoup
for a in the range from 0 to the length of html_list:
    if html_list[a] is a <h3> object named "sIdentification" and
html_list[a+1] is a <dl> object:
        fetched_id_list = html_list[a+1]
        for b in range from 0 to the length of fetched_id_list:
            if id_list[b] is a <dt> object with the value "Display Name" and
id_list[b+1] is a <dd> object:
                df.loc[i, "Display Name"] = id_list[b+1]
4.      Execute the function "fetch_data_for_id(i)" for i ranging from 0 to 40000
5.      Save df to csv file with pandas

```

H-statements_statistics

Dataset	Descriptor	Significance level	Balanced accuracy	Accuracy	Sensitivity	Specificity	MCC	ROC_auc ^a
H30x012345	consensus_cls_all	0.1	0.8688	0.8684	0.8654	0.8723	0.7349	NA
H30x012345	consensus_cls_all	0.15	0.8222	0.8228	0.826	0.8183	0.6399	NA
H30x012345	consensus_cls_all	0.2	0.7902	0.791	0.7948	0.7855	0.5747	NA
H30x012345	consensus_cls_all	0.25	0.7836	0.7864	0.7992	0.768	0.5629	NA
H30x012345	consensus_cls_all	0.3	0.7857	0.7883	0.8	0.7714	0.5672	NA
H30x012345	consensus_pvals_all	0.1	0.8839	0.8837	0.8816	0.8862	0.7656	0.9210
H30x012345	consensus_pvals_all	0.15	0.8503	0.8508	0.8536	0.847	0.6971	0.9094
H30x012345	consensus_pvals_all	0.2	0.8178	0.8183	0.8205	0.8151	0.6306	0.8990
H30x012345	consensus_pvals_all	0.25	0.7853	0.7863	0.7909	0.7797	0.5649	0.8894
H30x012345	consensus_pvals_all	0.3	0.8076	0.8094	0.8179	0.7974	0.6111	0.8862
H30x012345	core-substituent_fps	0.1	0.8236	0.8235	0.823	0.8242	0.6428	0.8624
H30x012345	core-substituent_fps	0.15	0.7906	0.7905	0.7902	0.791	0.575	0.8523
H30x012345	core-substituent_fps	0.2	0.7633	0.7634	0.7636	0.7631	0.5207	0.8424
H30x012345	core-substituent_fps	0.25	0.7375	0.7374	0.7366	0.7385	0.469	0.8331
H30x012345	core-substituent_fps	0.3	0.7483	0.7485	0.749	0.7477	0.4907	0.8291
H30x012345	deepsmls_4_hashed_1024	0.1	0.8309	0.8298	0.8228	0.839	0.6579	0.8760
H30x012345	deepsmls_4_hashed_1024	0.15	0.7992	0.7989	0.7973	0.801	0.5932	0.8651
H30x012345	deepsmls_4_hashed_1024	0.2	0.7662	0.766	0.7648	0.7676	0.5267	0.8547
H30x012345	deepsmls_4_hashed_1024	0.25	0.7419	0.7425	0.7454	0.7384	0.478	0.8455
H30x012345	deepsmls_4_hashed_1024	0.3	0.7572	0.7583	0.7634	0.751	0.5089	0.8421
H30x012345	morgan2_hashed_1024	0.1	0.8367	0.8349	0.8229	0.8505	0.6689	0.8892
H30x012345	morgan2_hashed_1024	0.15	0.8076	0.8065	0.8011	0.814	0.6094	0.8775
H30x012345	morgan2_hashed_1024	0.2	0.781	0.7807	0.779	0.7831	0.5559	0.8678
H30x012345	morgan2_hashed_1024	0.25	0.769	0.7693	0.7705	0.7675	0.5318	0.8613
H30x012345	morgan2_hashed_1024	0.3	0.7896	0.7908	0.7966	0.7826	0.5743	0.8601
H30x012345	morgan4_hashed_1024	0.1	0.8361	0.8344	0.8195	0.8528	0.669	0.8774
H30x012345	morgan4_hashed_1024	0.15	0.8039	0.8031	0.7989	0.8089	0.6031	0.8675
H30x012345	morgan4_hashed_1024	0.2	0.7764	0.7761	0.7749	0.7779	0.5472	0.8584
H30x012345	morgan4_hashed_1024	0.25	0.7608	0.7608	0.7608	0.7609	0.5155	0.8510
H30x012345	morgan4_hashed_1024	0.3	0.7806	0.7821	0.7891	0.7721	0.5567	0.8491
H30x012345	ngram_4_hashed_1024	0.1	0.8354	0.8346	0.8287	0.8422	0.667	0.8835
H30x012345	ngram_4_hashed_1024	0.15	0.8056	0.8051	0.8024	0.8088	0.6058	0.8721
H30x012345	ngram_4_hashed_1024	0.2	0.7748	0.7748	0.7746	0.7751	0.5441	0.8623
H30x012345	ngram_4_hashed_1024	0.25	0.749	0.7499	0.7538	0.7442	0.4923	0.8531
H30x012345	ngram_4_hashed_1024	0.3	0.7671	0.768	0.7724	0.7617	0.5289	0.8500
H30x012345	ngram_4_hashed_256	0.1	0.8375	0.8363	0.8277	0.8472	0.6715	0.8848
H30x012345	ngram_4_hashed_256	0.15	0.7986	0.7972	0.7896	0.8075	0.5916	0.8731
H30x012345	ngram_4_hashed_256	0.2	0.7673	0.7658	0.7588	0.7758	0.5279	0.8623
H30x012345	ngram_4_hashed_256	0.25	0.7458	0.7458	0.7456	0.7461	0.4854	0.8526
H30x012345	ngram_4_hashed_256	0.3	0.7633	0.7639	0.7668	0.7598	0.5211	0.8496
H30x012345	ngram_4_hashed_64	0.1	0.8406	0.8403	0.8384	0.8428	0.6775	0.8792
H30x012345	ngram_4_hashed_64	0.15	0.8061	0.8056	0.8031	0.809	0.6063	0.8687
H30x012345	ngram_4_hashed_64	0.2	0.774	0.774	0.7743	0.7736	0.5418	0.8589
H30x012345	ngram_4_hashed_64	0.25	0.7473	0.7476	0.749	0.7456	0.4885	0.8501
H30x012345	ngram_4_hashed_64	0.3	0.7641	0.7653	0.7708	0.7575	0.523	0.8465
H30x012345	ngram_6_hashed_1024	0.1	0.8243	0.8226	0.8098	0.8387	0.645	0.8707
H30x012345	ngram_6_hashed_1024	0.15	0.7951	0.7937	0.7851	0.8052	0.5855	0.8597
H30x012345	ngram_6_hashed_1024	0.2	0.7666	0.7646	0.7548	0.7785	0.5268	0.8499
H30x012345	ngram_6_hashed_1024	0.25	0.7451	0.7436	0.737	0.7532	0.4833	0.8413

H30x012345	ngram_6_hashed_1024	0.3	0.7625	0.7625	0.7625	0.7625	0.5192	0.8385
H30x012345	ngram_6_hashed_256	0.1	0.8221	0.8197	0.7993	0.8448	0.6407	0.8684
H30x012345	ngram_6_hashed_256	0.15	0.7935	0.7914	0.7797	0.8072	0.5813	0.8579
H30x012345	ngram_6_hashed_256	0.2	0.7652	0.7634	0.7553	0.775	0.5236	0.8482
H30x012345	ngram_6_hashed_256	0.25	0.7399	0.7384	0.7317	0.7481	0.4731	0.8392
H30x012345	ngram_6_hashed_256	0.3	0.749	0.7484	0.7454	0.7527	0.4915	0.8353
H30x012345	ngram_6_hashed_64	0.1	0.8268	0.8258	0.8208	0.8328	0.6482	0.8699
H30x012345	ngram_6_hashed_64	0.15	0.7915	0.7904	0.7849	0.7981	0.5769	0.8587
H30x012345	ngram_6_hashed_64	0.2	0.7635	0.7622	0.7564	0.7706	0.5204	0.8485
H30x012345	ngram_6_hashed_64	0.25	0.7392	0.7375	0.7301	0.7482	0.4716	0.8393
H30x012345	ngram_6_hashed_64	0.3	0.7561	0.7547	0.7485	0.7637	0.5055	0.8358
H30x012345	ngramsPE_4_hashed_1024	0.1	0.8287	0.8271	0.8131	0.8443	0.6545	0.8736
H30x012345	ngramsPE_4_hashed_1024	0.15	0.798	0.7966	0.7877	0.8083	0.5914	0.8629
H30x012345	ngramsPE_4_hashed_1024	0.2	0.7707	0.7692	0.762	0.7794	0.5352	0.8523
H30x012345	ngramsPE_4_hashed_1024	0.25	0.7475	0.7473	0.746	0.7491	0.4888	0.8432
H30x012345	ngramsPE_4_hashed_1024	0.3	0.7629	0.7633	0.7649	0.7609	0.52	0.8397
H30x012345	SMILES_extnd_connect_fps_2_1024	0.1	0.8424	0.8423	0.8419	0.8428	0.6794	0.8753
H30x012345	SMILES_extnd_connect_fps_2_1024	0.15	0.809	0.8091	0.81	0.808	0.6122	0.8667
H30x012345	SMILES_extnd_connect_fps_2_1024	0.2	0.7781	0.7775	0.7746	0.7816	0.5496	0.8586
H30x012345	SMILES_extnd_connect_fps_2_1024	0.25	0.7555	0.7558	0.7568	0.7542	0.5052	0.8509
H30x012345	SMILES_extnd_connect_fps_2_1024	0.3	0.776	0.7765	0.7787	0.7733	0.5462	0.8486
H30x012345	SMILES_extnd_connect_fps_4_1024	0.1	0.8377	0.8371	0.8333	0.8421	0.6708	0.8806
H30x012345	SMILES_extnd_connect_fps_4_1024	0.15	0.8049	0.8048	0.8039	0.8059	0.6047	0.8701
H30x012345	SMILES_extnd_connect_fps_4_1024	0.2	0.7782	0.7785	0.7803	0.776	0.5506	0.8609
H30x012345	SMILES_extnd_connect_fps_4_1024	0.25	0.7598	0.7596	0.7586	0.761	0.5134	0.8535
H30x012345	SMILES_extnd_connect_fps_4_1024	0.3	0.786	0.7875	0.7944	0.7777	0.5673	0.8520
H30x012345	selfies_4_hashed_1024	0.1	0.8269	0.8257	0.8164	0.8374	0.6504	0.8651
H30x012345	selfies_4_hashed_1024	0.15	0.7951	0.7951	0.7949	0.7954	0.5858	0.8547
H30x012345	selfies_4_hashed_1024	0.2	0.7699	0.7699	0.7701	0.7697	0.5342	0.8453
H30x012345	selfies_4_hashed_1024	0.25	0.7442	0.7447	0.7473	0.7411	0.4827	0.8366
H30x012345	selfies_4_hashed_1024	0.3	0.7506	0.7523	0.7603	0.7408	0.4962	0.8323
H31x0123	consensus_cls_all	0.1	0.8667	0.8617	0.8744	0.859	0.6257	NA
H31x0123	consensus_cls_all	0.15	0.8256	0.817	0.8382	0.813	0.5264	NA
H31x0123	consensus_cls_all	0.2	0.7871	0.7758	0.8035	0.7707	0.4458	NA
H31x0123	consensus_cls_all	0.25	0.775	0.7626	0.7929	0.7572	0.4214	NA
H31x0123	consensus_cls_all	0.3	0.7775	0.7663	0.7936	0.7613	0.4265	NA
H31x0123	consensus_pvals_all	0.1	0.8886	0.8805	0.901	0.8762	0.6695	0.9302
H31x0123	consensus_pvals_all	0.15	0.8528	0.8456	0.8633	0.8422	0.5841	0.9174
H31x0123	consensus_pvals_all	0.2	0.8195	0.8151	0.8259	0.8131	0.5125	0.9062
H31x0123	consensus_pvals_all	0.25	0.7862	0.7813	0.7932	0.7791	0.4463	0.8952
H31x0123	consensus_pvals_all	0.3	0.7931	0.7919	0.7948	0.7914	0.4624	0.8894
H31x0123	core-substituent_fps	0.1	0.8158	0.8041	0.8333	0.7983	0.509	0.8556
H31x0123	core-substituent_fps	0.15	0.7781	0.7723	0.7868	0.7694	0.4429	0.8438
H31x0123	core-substituent_fps	0.2	0.7569	0.7563	0.7578	0.756	0.4021	0.8335
H31x0123	core-substituent_fps	0.25	0.7417	0.7396	0.7446	0.7387	0.3699	0.8246
H31x0123	core-substituent_fps	0.3	0.7428	0.7451	0.7395	0.7462	0.3725	0.8199
H31x0123	deepsmiles_4_hashed_1024	0.1	0.8369	0.8209	0.8609	0.813	0.5462	0.8896
H31x0123	deepsmiles_4_hashed_1024	0.15	0.7963	0.7852	0.8126	0.7799	0.4682	0.8752
H31x0123	deepsmiles_4_hashed_1024	0.2	0.7674	0.7574	0.782	0.7528	0.412	0.8629
H31x0123	deepsmiles_4_hashed_1024	0.25	0.7375	0.7339	0.7427	0.7323	0.3603	0.8511
H31x0123	deepsmiles_4_hashed_1024	0.3	0.7361	0.7389	0.7321	0.7401	0.359	0.8441
H31x0123	morgan2_hashed_1024	0.1	0.845	0.8384	0.8549	0.8351	0.5734	0.8904
H31x0123	morgan2_hashed_1024	0.15	0.8063	0.8016	0.8132	0.7994	0.4912	0.8791

H31x0123	morgan2_hashed_1024	0.2	0.7759	0.7711	0.7829	0.7689	0.4292	0.8692
H31x0123	morgan2_hashed_1024	0.25	0.7493	0.75	0.7483	0.7503	0.3825	0.8601
H31x0123	morgan2_hashed_1024	0.3	0.7731	0.7726	0.774	0.7723	0.4249	0.8575
H31x0123	morgan4_hashed_1024	0.1	0.8319	0.8289	0.8364	0.8274	0.542	0.8822
H31x0123	morgan4_hashed_1024	0.15	0.8008	0.7976	0.8054	0.7962	0.4782	0.8703
H31x0123	morgan4_hashed_1024	0.2	0.7706	0.7648	0.7791	0.7622	0.4189	0.8599
H31x0123	morgan4_hashed_1024	0.25	0.7489	0.7436	0.7565	0.7412	0.3786	0.8507
H31x0123	morgan4_hashed_1024	0.3	0.7624	0.7595	0.7665	0.7583	0.4026	0.8472
H31x0123	ngram_4_hashed_1024	0.1	0.8305	0.8321	0.8281	0.8329	0.5484	0.8704
H31x0123	ngram_4_hashed_1024	0.15	0.7971	0.794	0.8017	0.7925	0.4731	0.8600
H31x0123	ngram_4_hashed_1024	0.2	0.7718	0.7676	0.7778	0.7658	0.4236	0.8507
H31x0123	ngram_4_hashed_1024	0.25	0.7414	0.7388	0.7452	0.7377	0.3679	0.8418
H31x0123	ngram_4_hashed_1024	0.3	0.7522	0.7485	0.7575	0.7468	0.3861	0.8376
H31x0123	ngram_4_hashed_256	0.1	0.8259	0.8176	0.8383	0.8135	0.5327	0.8745
H31x0123	ngram_4_hashed_256	0.15	0.7954	0.7897	0.8038	0.787	0.4696	0.8625
H31x0123	ngram_4_hashed_256	0.2	0.7629	0.7563	0.7724	0.7533	0.4074	0.8519
H31x0123	ngram_4_hashed_256	0.25	0.7374	0.7347	0.7413	0.7335	0.3634	0.8417
H31x0123	ngram_4_hashed_256	0.3	0.7399	0.7397	0.7401	0.7397	0.3662	0.8361
H31x0123	ngram_4_hashed_64	0.1	0.823	0.8181	0.8302	0.8158	0.5234	0.8648
H31x0123	ngram_4_hashed_64	0.15	0.7951	0.79	0.8025	0.7877	0.4677	0.8543
H31x0123	ngram_4_hashed_64	0.2	0.7713	0.7646	0.7809	0.7617	0.417	0.8459
H31x0123	ngram_4_hashed_64	0.25	0.7438	0.7408	0.748	0.7395	0.3716	0.8375
H31x0123	ngram_4_hashed_64	0.3	0.7489	0.748	0.7502	0.7476	0.3805	0.8331
H31x0123	ngram_6_hashed_1024	0.1	0.8297	0.8234	0.8389	0.8204	0.5384	0.8680
H31x0123	ngram_6_hashed_1024	0.15	0.7982	0.7948	0.8032	0.7932	0.4778	0.8568
H31x0123	ngram_6_hashed_1024	0.2	0.7686	0.7634	0.7761	0.7611	0.4173	0.8475
H31x0123	ngram_6_hashed_1024	0.25	0.7498	0.744	0.7583	0.7414	0.3819	0.8390
H31x0123	ngram_6_hashed_1024	0.3	0.7491	0.7457	0.754	0.7442	0.381	0.8342
H31x0123	ngram_6_hashed_256	0.1	0.8251	0.8224	0.8291	0.8211	0.5296	0.8543
H31x0123	ngram_6_hashed_256	0.15	0.7946	0.7898	0.8015	0.7877	0.465	0.8462
H31x0123	ngram_6_hashed_256	0.2	0.7682	0.7584	0.7823	0.754	0.4118	0.8383
H31x0123	ngram_6_hashed_256	0.25	0.7408	0.7327	0.7524	0.7292	0.3645	0.8303
H31x0123	ngram_6_hashed_256	0.3	0.7448	0.7396	0.7522	0.7374	0.3715	0.8260
H31x0123	ngram_6_hashed_64	0.1	0.8278	0.8114	0.8526	0.803	0.533	0.8647
H31x0123	ngram_6_hashed_64	0.15	0.7945	0.7789	0.8177	0.7713	0.4638	0.8551
H31x0123	ngram_6_hashed_64	0.2	0.7581	0.7484	0.7723	0.744	0.3975	0.8456
H31x0123	ngram_6_hashed_64	0.25	0.737	0.7284	0.7495	0.7246	0.3585	0.8359
H31x0123	ngram_6_hashed_64	0.3	0.7288	0.7219	0.7386	0.7189	0.3449	0.8292
H31x0123	ngramsPE_4_hashed_1024	0.1	0.8198	0.815	0.8268	0.8127	0.5207	0.8717
H31x0123	ngramsPE_4_hashed_1024	0.15	0.7897	0.7817	0.8015	0.7779	0.4604	0.8600
H31x0123	ngramsPE_4_hashed_1024	0.2	0.7593	0.7507	0.7718	0.7468	0.4014	0.8490
H31x0123	ngramsPE_4_hashed_1024	0.25	0.7324	0.7252	0.743	0.7219	0.3521	0.8392
H31x0123	ngramsPE_4_hashed_1024	0.3	0.7255	0.7214	0.7313	0.7196	0.3407	0.8322
H31x0123	SMILES_extnd_connect_fps_2_1024	0.1	0.8415	0.8379	0.8467	0.8362	0.5649	0.8744
H31x0123	SMILES_extnd_connect_fps_2_1024	0.15	0.8068	0.8043	0.8105	0.8031	0.4902	0.8656
H31x0123	SMILES_extnd_connect_fps_2_1024	0.2	0.779	0.7765	0.7825	0.7754	0.4356	0.8569
H31x0123	SMILES_extnd_connect_fps_2_1024	0.25	0.7511	0.7551	0.7452	0.7569	0.388	0.8489
H31x0123	SMILES_extnd_connect_fps_2_1024	0.3	0.7667	0.7696	0.7625	0.7708	0.4169	0.8457
H31x0123	SMILES_extnd_connect_fps_4_1024	0.1	0.8367	0.8326	0.8427	0.8306	0.5536	0.8868
H31x0123	SMILES_extnd_connect_fps_4_1024	0.15	0.8102	0.8068	0.8151	0.8053	0.4921	0.8756
H31x0123	SMILES_extnd_connect_fps_4_1024	0.2	0.7783	0.778	0.7787	0.7779	0.4361	0.8649
H31x0123	SMILES_extnd_connect_fps_4_1024	0.25	0.7584	0.7594	0.757	0.7598	0.3981	0.8564
H31x0123	SMILES_extnd_connect_fps_4_1024	0.3	0.7768	0.7786	0.7742	0.7794	0.4317	0.8537

H31x0123	selfies_4_hashed_1024	0.1	0.8209	0.8196	0.8228	0.819	0.5318	0.8666
H31x0123	selfies_4_hashed_1024	0.15	0.7835	0.7786	0.7908	0.7762	0.4493	0.8549
H31x0123	selfies_4_hashed_1024	0.2	0.7533	0.7521	0.755	0.7515	0.393	0.8432
H31x0123	selfies_4_hashed_1024	0.25	0.7288	0.7261	0.7327	0.7249	0.348	0.8327
H31x0123	selfies_4_hashed_1024	0.3	0.7209	0.7199	0.7224	0.7194	0.334	0.8251
H31x57	consensus_cls_all	0.1	0.8433	0.8432	0.8452	0.8414	0.6855	NA
H31x57	consensus_cls_all	0.15	0.8016	0.8014	0.8048	0.7984	0.6027	NA
H31x57	consensus_cls_all	0.2	0.7653	0.765	0.7738	0.7569	0.5303	NA
H31x57	consensus_cls_all	0.25	0.7382	0.7377	0.7518	0.7246	0.476	NA
H31x57	consensus_cls_all	0.3	0.7342	0.7334	0.7548	0.7135	0.4681	NA
H31x57	consensus_pvals_all	0.1	0.8582	0.8584	0.8561	0.8603	0.7156	0.8873
H31x57	consensus_pvals_all	0.15	0.8239	0.824	0.8213	0.8265	0.6475	0.8758
H31x57	consensus_pvals_all	0.2	0.7933	0.7931	0.7977	0.7889	0.5862	0.8648
H31x57	consensus_pvals_all	0.25	0.765	0.7648	0.7716	0.7584	0.5297	0.8541
H31x57	consensus_pvals_all	0.3	0.7381	0.7379	0.7434	0.7327	0.4758	0.8440
H31x57	core-substituent_fps	0.1	0.7803	0.7806	0.7737	0.7869	0.5602	0.8128
H31x57	core-substituent_fps	0.15	0.7552	0.756	0.7431	0.7674	0.5103	0.8024
H31x57	core-substituent_fps	0.2	0.7234	0.7236	0.7203	0.7266	0.4465	0.7928
H31x57	core-substituent_fps	0.25	0.7004	0.7004	0.7006	0.7002	0.4004	0.7832
H31x57	core-substituent_fps	0.3	0.6809	0.6808	0.683	0.6788	0.3614	0.7743
H31x57	deepsmls_4_hashed_1024	0.1	0.7995	0.7997	0.7961	0.8029	0.5985	0.8377
H31x57	deepsmls_4_hashed_1024	0.15	0.7668	0.7669	0.7645	0.7691	0.5332	0.8260
H31x57	deepsmls_4_hashed_1024	0.2	0.7394	0.7394	0.7392	0.7397	0.4784	0.8152
H31x57	deepsmls_4_hashed_1024	0.25	0.7177	0.7176	0.721	0.7145	0.4352	0.8054
H31x57	deepsmls_4_hashed_1024	0.3	0.6967	0.6966	0.6987	0.6947	0.3932	0.7966
H31x57	morgan2_hashed_1024	0.1	0.8176	0.818	0.8114	0.8237	0.6345	0.8591
H31x57	morgan2_hashed_1024	0.15	0.7839	0.7843	0.7758	0.792	0.5677	0.8476
H31x57	morgan2_hashed_1024	0.2	0.7601	0.7604	0.7526	0.7676	0.5201	0.8372
H31x57	morgan2_hashed_1024	0.25	0.736	0.7363	0.7296	0.7424	0.4718	0.8278
H31x57	morgan2_hashed_1024	0.3	0.7295	0.7297	0.7261	0.733	0.4588	0.8212
H31x57	morgan4_hashed_1024	0.1	0.8025	0.8035	0.7897	0.8153	0.6048	0.8418
H31x57	morgan4_hashed_1024	0.15	0.773	0.7738	0.7615	0.7845	0.5457	0.8309
H31x57	morgan4_hashed_1024	0.2	0.7501	0.7505	0.7428	0.7573	0.4998	0.8210
H31x57	morgan4_hashed_1024	0.25	0.7287	0.729	0.7234	0.734	0.4572	0.8122
H31x57	morgan4_hashed_1024	0.3	0.7139	0.714	0.7103	0.7175	0.4275	0.8050
H31x57	ngram_4_hashed_1024	0.1	0.7894	0.7903	0.7781	0.8008	0.5786	0.8262
H31x57	ngram_4_hashed_1024	0.15	0.7645	0.765	0.7555	0.7736	0.5289	0.8154
H31x57	ngram_4_hashed_1024	0.2	0.7388	0.7389	0.7355	0.7421	0.4773	0.8058
H31x57	ngram_4_hashed_1024	0.25	0.7157	0.7159	0.7113	0.7202	0.4313	0.7972
H31x57	ngram_4_hashed_1024	0.3	0.6975	0.6977	0.6916	0.7034	0.3949	0.7889
H31x57	ngram_4_hashed_256	0.1	0.7925	0.7928	0.787	0.798	0.5846	0.8224
H31x57	ngram_4_hashed_256	0.15	0.76	0.76	0.761	0.7591	0.5195	0.8117
H31x57	ngram_4_hashed_256	0.2	0.7357	0.7356	0.7374	0.734	0.471	0.8025
H31x57	ngram_4_hashed_256	0.25	0.7176	0.7176	0.7191	0.7162	0.4349	0.7938
H31x57	ngram_4_hashed_256	0.3	0.6972	0.6971	0.6989	0.6954	0.394	0.7859
H31x57	ngram_4_hashed_64	0.1	0.7751	0.7753	0.771	0.7791	0.5497	0.8082
H31x57	ngram_4_hashed_64	0.15	0.7477	0.7476	0.7498	0.7455	0.4949	0.7979
H31x57	ngram_4_hashed_64	0.2	0.7286	0.7285	0.7301	0.7271	0.4568	0.7887
H31x57	ngram_4_hashed_64	0.25	0.7084	0.7085	0.7062	0.7106	0.4166	0.7804
H31x57	ngram_4_hashed_64	0.3	0.6881	0.6881	0.689	0.6872	0.376	0.7724
H31x57	ngram_6_hashed_1024	0.1	0.7945	0.7953	0.7843	0.8047	0.5884	0.8245
H31x57	ngram_6_hashed_1024	0.15	0.7645	0.7647	0.7619	0.7672	0.5285	0.8151
H31x57	ngram_6_hashed_1024	0.2	0.738	0.7381	0.7371	0.7389	0.4755	0.8060

H31x57	ngram_6_hashed_1024	0.25	0.7159	0.7159	0.7149	0.7169	0.4315	0.7973
H31x57	ngram_6_hashed_1024	0.3	0.6966	0.6966	0.6968	0.6963	0.3929	0.7891
H31x57	ngram_6_hashed_256	0.1	0.7919	0.7916	0.795	0.7887	0.5826	0.8201
H31x57	ngram_6_hashed_256	0.15	0.7594	0.7596	0.7568	0.7621	0.5185	0.8101
H31x57	ngram_6_hashed_256	0.2	0.7379	0.7378	0.7403	0.7356	0.4755	0.8012
H31x57	ngram_6_hashed_256	0.25	0.7132	0.7132	0.7124	0.714	0.4261	0.7925
H31x57	ngram_6_hashed_256	0.3	0.6953	0.6954	0.6946	0.6961	0.3904	0.7844
H31x57	ngram_6_hashed_64	0.1	0.7861	0.7859	0.7895	0.7827	0.5716	0.8197
H31x57	ngram_6_hashed_64	0.15	0.7588	0.7585	0.7664	0.7513	0.5172	0.8089
H31x57	ngram_6_hashed_64	0.2	0.732	0.7318	0.7382	0.7259	0.4638	0.7989
H31x57	ngram_6_hashed_64	0.25	0.7106	0.7104	0.7172	0.7041	0.421	0.7899
H31x57	ngram_6_hashed_64	0.3	0.6929	0.6927	0.6976	0.6882	0.3855	0.7814
H31x57	ngramsPE_4_hashed_1024	0.1	0.7934	0.7939	0.7869	0.7999	0.5859	0.8321
H31x57	ngramsPE_4_hashed_1024	0.15	0.7635	0.764	0.7545	0.7725	0.5267	0.8207
H31x57	ngramsPE_4_hashed_1024	0.2	0.7387	0.7389	0.7334	0.7439	0.477	0.8100
H31x57	ngramsPE_4_hashed_1024	0.25	0.7185	0.7186	0.7175	0.7196	0.4367	0.8007
H31x57	ngramsPE_4_hashed_1024	0.3	0.6996	0.6996	0.7002	0.699	0.3989	0.7925
H31x57	SMILES_extnd_connect_fps_2_1024	0.1	0.7973	0.7973	0.7965	0.7981	0.5944	0.8335
H31x57	SMILES_extnd_connect_fps_2_1024	0.15	0.7687	0.7685	0.7718	0.7655	0.537	0.8229
H31x57	SMILES_extnd_connect_fps_2_1024	0.2	0.7432	0.7431	0.7454	0.741	0.4861	0.8133
H31x57	SMILES_extnd_connect_fps_2_1024	0.25	0.7175	0.7174	0.7179	0.7171	0.4347	0.8043
H31x57	SMILES_extnd_connect_fps_2_1024	0.3	0.6995	0.6994	0.7002	0.6987	0.3987	0.7962
H31x57	SMILES_extnd_connect_fps_4_1024	0.1	0.8054	0.8055	0.802	0.8088	0.6107	0.8505
H31x57	SMILES_extnd_connect_fps_4_1024	0.15	0.7791	0.779	0.7829	0.7754	0.5579	0.8381
H31x57	SMILES_extnd_connect_fps_4_1024	0.2	0.7541	0.754	0.7578	0.7504	0.5079	0.8276
H31x57	SMILES_extnd_connect_fps_4_1024	0.25	0.729	0.729	0.7284	0.7295	0.4576	0.8179
H31x57	SMILES_extnd_connect_fps_4_1024	0.3	0.7098	0.7098	0.7104	0.7092	0.4193	0.8093
H31x57	selfies_4_hashed_1024	0.1	0.7905	0.7909	0.784	0.797	0.5806	0.8229
H31x57	selfies_4_hashed_1024	0.15	0.7622	0.7625	0.7554	0.7689	0.524	0.8126
H31x57	selfies_4_hashed_1024	0.2	0.7386	0.7386	0.738	0.7392	0.4769	0.8035
H31x57	selfies_4_hashed_1024	0.25	0.7148	0.7147	0.7174	0.7121	0.4292	0.7949
H31x57	selfies_4_hashed_1024	0.3	0.6951	0.695	0.6978	0.6924	0.39	0.7868
H33x0123	consensus_cls_all	0.1	0.8808	0.846	0.9206	0.8411	0.4523	NA
H33x0123	consensus_cls_all	0.15	0.822	0.7998	0.8467	0.7972	0.3359	NA
H33x0123	consensus_cls_all	0.2	0.782	0.7584	0.8079	0.756	0.2675	NA
H33x0123	consensus_cls_all	0.25	0.7692	0.7398	0.8015	0.7369	0.2468	NA
H33x0123	consensus_cls_all	0.3	0.7711	0.7411	0.8041	0.7381	0.2475	NA
H33x0123	consensus_pvals_all	0.1	0.9027	0.8659	0.9448	0.8607	0.4957	0.9327
H33x0123	consensus_pvals_all	0.15	0.869	0.8401	0.9009	0.837	0.397	0.9254
H33x0123	consensus_pvals_all	0.2	0.8189	0.8089	0.8299	0.8079	0.3251	0.9121
H33x0123	consensus_pvals_all	0.25	0.7927	0.7835	0.8029	0.7825	0.2841	0.8982
H33x0123	consensus_pvals_all	0.3	0.7787	0.7646	0.7941	0.7633	0.2603	0.8862
H33x0123	core-substituent_fps	0.1	0.733	0.7387	0.7267	0.7393	0.2229	0.7700
H33x0123	core-substituent_fps	0.15	0.7171	0.7243	0.7091	0.725	0.1954	0.7638
H33x0123	core-substituent_fps	0.2	0.7073	0.7117	0.7025	0.7121	0.1856	0.7554
H33x0123	core-substituent_fps	0.25	0.6863	0.6956	0.676	0.6965	0.1633	0.7482
H33x0123	core-substituent_fps	0.3	0.6769	0.6854	0.6676	0.6862	0.1545	0.7415
H33x0123	deepsmiles_4_hashed_1024	0.1	0.7947	0.7753	0.8164	0.7729	0.304	0.8321
H33x0123	deepsmiles_4_hashed_1024	0.15	0.7554	0.7451	0.7668	0.744	0.2437	0.8218
H33x0123	deepsmiles_4_hashed_1024	0.2	0.731	0.7221	0.7407	0.7212	0.2126	0.8103
H33x0123	deepsmiles_4_hashed_1024	0.25	0.7036	0.7007	0.7067	0.7004	0.1811	0.7992
H33x0123	deepsmiles_4_hashed_1024	0.3	0.6959	0.6912	0.7011	0.6907	0.173	0.7896
H33x0123	morgan2_hashed_1024	0.1	0.7718	0.7628	0.7821	0.7616	0.29	0.8108

H33x0123	morgan2_hashed_1024	0.15	0.7625	0.7527	0.7735	0.7515	0.2629	0.8019
H33x0123	morgan2_hashed_1024	0.2	0.7378	0.7274	0.7492	0.7263	0.2228	0.7956
H33x0123	morgan2_hashed_1024	0.25	0.7196	0.7117	0.7283	0.7109	0.2001	0.7894
H33x0123	morgan2_hashed_1024	0.3	0.7087	0.7025	0.7154	0.7019	0.1854	0.7841
H33x0123	morgan4_hashed_1024	0.1	0.7589	0.7398	0.7806	0.7373	0.2667	0.8071
H33x0123	morgan4_hashed_1024	0.15	0.7392	0.7216	0.7589	0.7195	0.2336	0.7950
H33x0123	morgan4_hashed_1024	0.2	0.7248	0.6969	0.7559	0.6937	0.2106	0.7853
H33x0123	morgan4_hashed_1024	0.25	0.7084	0.687	0.7319	0.6848	0.1877	0.7776
H33x0123	morgan4_hashed_1024	0.3	0.6841	0.6793	0.6894	0.6788	0.1622	0.7704
H33x0123	ngram_4_hashed_1024	0.1	0.7889	0.7576	0.8246	0.7533	0.304	0.8265
H33x0123	ngram_4_hashed_1024	0.15	0.7604	0.7485	0.7739	0.747	0.2592	0.8169
H33x0123	ngram_4_hashed_1024	0.2	0.739	0.744	0.7335	0.7445	0.2279	0.8066
H33x0123	ngram_4_hashed_1024	0.25	0.7167	0.7296	0.7026	0.7309	0.2011	0.7970
H33x0123	ngram_4_hashed_1024	0.3	0.7154	0.7272	0.7023	0.7284	0.1973	0.7909
H33x0123	ngram_4_hashed_256	0.1	0.7935	0.7695	0.8206	0.7663	0.3095	0.8352
H33x0123	ngram_4_hashed_256	0.15	0.7547	0.7465	0.7638	0.7455	0.2496	0.8231
H33x0123	ngram_4_hashed_256	0.2	0.7175	0.7212	0.7134	0.7216	0.2029	0.8114
H33x0123	ngram_4_hashed_256	0.25	0.7006	0.7062	0.6944	0.7067	0.1829	0.7998
H33x0123	ngram_4_hashed_256	0.3	0.682	0.6929	0.6701	0.6939	0.1621	0.7902
H33x0123	ngram_4_hashed_64	0.1	0.7854	0.7591	0.8148	0.7559	0.2917	0.8269
H33x0123	ngram_4_hashed_64	0.15	0.7607	0.7385	0.7854	0.736	0.2499	0.8181
H33x0123	ngram_4_hashed_64	0.2	0.7385	0.7177	0.7614	0.7155	0.2198	0.8091
H33x0123	ngram_4_hashed_64	0.25	0.7211	0.7054	0.7384	0.7039	0.1964	0.8005
H33x0123	ngram_4_hashed_64	0.3	0.7024	0.6934	0.7124	0.6925	0.1783	0.7929
H33x0123	ngram_6_hashed_1024	0.1	0.794	0.7764	0.8139	0.7741	0.3116	0.8400
H33x0123	ngram_6_hashed_1024	0.15	0.7672	0.757	0.7786	0.7558	0.2657	0.8284
H33x0123	ngram_6_hashed_1024	0.2	0.7427	0.7355	0.7508	0.7347	0.2303	0.8185
H33x0123	ngram_6_hashed_1024	0.25	0.7139	0.7227	0.7041	0.7236	0.1962	0.8085
H33x0123	ngram_6_hashed_1024	0.3	0.7099	0.7219	0.6966	0.7231	0.1918	0.8015
H33x0123	ngram_6_hashed_256	0.1	0.81	0.7866	0.8364	0.7837	0.3232	0.8552
H33x0123	ngram_6_hashed_256	0.15	0.7788	0.7623	0.797	0.7605	0.27	0.8436
H33x0123	ngram_6_hashed_256	0.2	0.7491	0.7357	0.7638	0.7344	0.2293	0.8334
H33x0123	ngram_6_hashed_256	0.25	0.7166	0.7184	0.7147	0.7185	0.1954	0.8229
H33x0123	ngram_6_hashed_256	0.3	0.7061	0.7052	0.7071	0.7051	0.1829	0.8142
H33x0123	ngram_6_hashed_64	0.1	0.7789	0.7525	0.8088	0.749	0.291	0.8308
H33x0123	ngram_6_hashed_64	0.15	0.7547	0.7359	0.7755	0.7338	0.2442	0.8191
H33x0123	ngram_6_hashed_64	0.2	0.7294	0.7281	0.7309	0.7279	0.2143	0.8061
H33x0123	ngram_6_hashed_64	0.25	0.7094	0.7092	0.7097	0.7092	0.1897	0.7951
H33x0123	ngram_6_hashed_64	0.3	0.6877	0.6915	0.6834	0.6919	0.1665	0.7854
H33x0123	ngramsPE_4_hashed_1024	0.1	0.7752	0.7723	0.7783	0.772	0.2822	0.8320
H33x0123	ngramsPE_4_hashed_1024	0.15	0.7462	0.7545	0.7371	0.7554	0.2406	0.8165
H33x0123	ngramsPE_4_hashed_1024	0.2	0.7214	0.7302	0.7117	0.7311	0.2017	0.8041
H33x0123	ngramsPE_4_hashed_1024	0.25	0.7091	0.7028	0.716	0.7022	0.1847	0.7928
H33x0123	ngramsPE_4_hashed_1024	0.3	0.6873	0.6871	0.6875	0.687	0.1636	0.7827
H33x0123	SMILES_extnd_connect_fps_2_1024	0.1	0.8292	0.8185	0.8411	0.8172	0.3563	0.8649
H33x0123	SMILES_extnd_connect_fps_2_1024	0.15	0.8035	0.793	0.8152	0.7919	0.304	0.8569
H33x0123	SMILES_extnd_connect_fps_2_1024	0.2	0.7747	0.7692	0.7807	0.7686	0.2603	0.8493
H33x0123	SMILES_extnd_connect_fps_2_1024	0.25	0.7443	0.7457	0.7428	0.7458	0.2269	0.8421
H33x0123	SMILES_extnd_connect_fps_2_1024	0.3	0.7549	0.7606	0.7486	0.7612	0.2412	0.8388
H33x0123	SMILES_extnd_connect_fps_4_1024	0.1	0.8283	0.8331	0.8228	0.8337	0.355	0.8699
H33x0123	SMILES_extnd_connect_fps_4_1024	0.15	0.7987	0.7988	0.7987	0.7988	0.3005	0.8599
H33x0123	SMILES_extnd_connect_fps_4_1024	0.2	0.7693	0.7679	0.7708	0.7678	0.2582	0.8506
H33x0123	SMILES_extnd_connect_fps_4_1024	0.25	0.748	0.7444	0.752	0.744	0.2308	0.8425

H33x0123	SMILES_extnd_connect_fps_4_1024	0.3	0.754	0.7527	0.7554	0.7526	0.2371	0.8386
H33x0123	selfies_4_hashed_1024	0.1	0.7739	0.7651	0.7837	0.7641	0.281	0.8082
H33x0123	selfies_4_hashed_1024	0.15	0.7416	0.745	0.7379	0.7454	0.2329	0.7988
H33x0123	selfies_4_hashed_1024	0.2	0.7194	0.7196	0.7193	0.7196	0.1997	0.7894
H33x0123	selfies_4_hashed_1024	0.25	0.6915	0.6982	0.684	0.6989	0.1698	0.7801
H33x0123	selfies_4_hashed_1024	0.3	0.6689	0.6831	0.6533	0.6845	0.1494	0.7707
H33x45	consensus_cls_all	0.1	0.8652	0.8648	0.8691	0.8614	0.7284	NA
H33x45	consensus_cls_all	0.15	0.8151	0.815	0.8158	0.8143	0.6292	NA
H33x45	consensus_cls_all	0.2	0.7822	0.7811	0.7962	0.7681	0.5628	NA
H33x45	consensus_cls_all	0.25	0.771	0.7698	0.7868	0.7553	0.5404	NA
H33x45	consensus_cls_all	0.3	0.774	0.7724	0.7938	0.7541	0.5462	NA
H33x45	consensus_pvals_all	0.1	0.8792	0.8794	0.8766	0.8817	0.7569	0.9081
H33x45	consensus_pvals_all	0.15	0.8444	0.8443	0.8457	0.843	0.6873	0.8976
H33x45	consensus_pvals_all	0.2	0.8098	0.8091	0.817	0.8025	0.6177	0.8877
H33x45	consensus_pvals_all	0.25	0.7809	0.7805	0.7857	0.7761	0.5603	0.8784
H33x45	consensus_pvals_all	0.3	0.7862	0.7856	0.7933	0.779	0.5707	0.8737
H33x45	core-substituent_fps	0.1	0.8058	0.8053	0.8111	0.8004	0.6097	0.8473
H33x45	core-substituent_fps	0.15	0.7779	0.777	0.7877	0.7681	0.5538	0.8339
H33x45	core-substituent_fps	0.2	0.7565	0.7557	0.7652	0.7477	0.5111	0.8236
H33x45	core-substituent_fps	0.25	0.732	0.731	0.7445	0.7196	0.4625	0.8147
H33x45	core-substituent_fps	0.3	0.7282	0.7268	0.7448	0.7115	0.4549	0.8088
H33x45	deepsmls_4_hashed_1024	0.1	0.8172	0.8181	0.8095	0.8248	0.632	0.8628
H33x45	deepsmls_4_hashed_1024	0.15	0.7892	0.7893	0.7884	0.79	0.5765	0.8503
H33x45	deepsmls_4_hashed_1024	0.2	0.7686	0.7685	0.7695	0.7677	0.5356	0.8406
H33x45	deepsmls_4_hashed_1024	0.25	0.7397	0.7395	0.7425	0.7368	0.4782	0.8317
H33x45	deepsmls_4_hashed_1024	0.3	0.7499	0.7499	0.7502	0.7496	0.4984	0.8275
H33x45	morgan2_hashed_1024	0.1	0.8409	0.8401	0.8523	0.8294	0.6803	0.8779
H33x45	morgan2_hashed_1024	0.15	0.8057	0.8053	0.8116	0.7999	0.6103	0.8682
H33x45	morgan2_hashed_1024	0.2	0.7785	0.7782	0.7821	0.7748	0.5556	0.8598
H33x45	morgan2_hashed_1024	0.25	0.7579	0.758	0.7566	0.7593	0.5148	0.8523
H33x45	morgan2_hashed_1024	0.3	0.7785	0.7784	0.7795	0.7775	0.5558	0.8505
H33x45	morgan4_hashed_1024	0.1	0.8283	0.8292	0.819	0.8376	0.6557	0.8650
H33x45	morgan4_hashed_1024	0.15	0.8023	0.8025	0.7989	0.8056	0.6035	0.8553
H33x45	morgan4_hashed_1024	0.2	0.7736	0.7738	0.7708	0.7764	0.5461	0.8473
H33x45	morgan4_hashed_1024	0.25	0.7506	0.7506	0.7507	0.7504	0.5001	0.8399
H33x45	morgan4_hashed_1024	0.3	0.767	0.767	0.7666	0.7674	0.533	0.8373
H33x45	ngram_4_hashed_1024	0.1	0.8233	0.825	0.8076	0.839	0.6462	0.8602
H33x45	ngram_4_hashed_1024	0.15	0.7939	0.7956	0.7772	0.8106	0.5874	0.8500
H33x45	ngram_4_hashed_1024	0.2	0.7645	0.7655	0.7532	0.7758	0.5283	0.8406
H33x45	ngram_4_hashed_1024	0.25	0.7426	0.7435	0.7305	0.7548	0.4848	0.8322
H33x45	ngram_4_hashed_1024	0.3	0.7546	0.7554	0.746	0.7633	0.5083	0.8287
H33x45	ngram_4_hashed_256	0.1	0.8127	0.8133	0.8087	0.8168	0.6226	0.8371
H33x45	ngram_4_hashed_256	0.15	0.7818	0.7825	0.7746	0.789	0.5623	0.8294
H33x45	ngram_4_hashed_256	0.2	0.7602	0.7605	0.7568	0.7636	0.5187	0.8217
H33x45	ngram_4_hashed_256	0.25	0.7447	0.7445	0.7474	0.742	0.4883	0.8149
H33x45	ngram_4_hashed_256	0.3	0.7521	0.7514	0.7612	0.743	0.5027	0.8116
H33x45	ngram_4_hashed_64	0.1	0.8173	0.8155	0.8333	0.8013	0.631	0.8454
H33x45	ngram_4_hashed_64	0.15	0.779	0.7789	0.7801	0.7779	0.5559	0.8350
H33x45	ngram_4_hashed_64	0.2	0.7514	0.7519	0.7461	0.7567	0.5018	0.8255
H33x45	ngram_4_hashed_64	0.25	0.7279	0.7278	0.7291	0.7267	0.4545	0.8165
H33x45	ngram_4_hashed_64	0.3	0.7335	0.7333	0.7361	0.7309	0.4657	0.8116
H33x45	ngram_6_hashed_1024	0.1	0.8149	0.8148	0.8154	0.8143	0.6271	0.8443
H33x45	ngram_6_hashed_1024	0.15	0.7872	0.7873	0.7868	0.7877	0.573	0.8354

H33x45	ngram_6_hashed_1024	0.2	0.7626	0.7626	0.7629	0.7624	0.5239	0.8270
H33x45	ngram_6_hashed_1024	0.25	0.7379	0.7375	0.7424	0.7334	0.4746	0.8193
H33x45	ngram_6_hashed_1024	0.3	0.7443	0.7438	0.7519	0.7368	0.4874	0.8153
H33x45	ngram_6_hashed_256	0.1	0.8117	0.8117	0.8119	0.8114	0.6211	0.8349
H33x45	ngram_6_hashed_256	0.15	0.7885	0.7884	0.7892	0.7877	0.5747	0.8283
H33x45	ngram_6_hashed_256	0.2	0.7611	0.7611	0.7607	0.7615	0.5207	0.8216
H33x45	ngram_6_hashed_256	0.25	0.7285	0.7284	0.7296	0.7273	0.4556	0.8145
H33x45	ngram_6_hashed_256	0.3	0.7242	0.7242	0.7238	0.7245	0.4471	0.8096
H33x45	ngram_6_hashed_64	0.1	0.8121	0.8121	0.8123	0.812	0.6218	0.8406
H33x45	ngram_6_hashed_64	0.15	0.7828	0.7834	0.7776	0.7881	0.564	0.8319
H33x45	ngram_6_hashed_64	0.2	0.7498	0.7502	0.7456	0.754	0.4983	0.8234
H33x45	ngram_6_hashed_64	0.25	0.7288	0.7293	0.7233	0.7344	0.4566	0.8152
H33x45	ngram_6_hashed_64	0.3	0.7209	0.7214	0.7142	0.7276	0.441	0.8087
H33x45	ngramsPE_4_hashed_1024	0.1	0.8205	0.8201	0.8256	0.8154	0.6394	0.8588
H33x45	ngramsPE_4_hashed_1024	0.15	0.787	0.7873	0.7835	0.7904	0.5726	0.8458
H33x45	ngramsPE_4_hashed_1024	0.2	0.7628	0.7635	0.7548	0.7708	0.5247	0.8360
H33x45	ngramsPE_4_hashed_1024	0.25	0.7382	0.7389	0.7288	0.7476	0.4758	0.8275
H33x45	ngramsPE_4_hashed_1024	0.3	0.7327	0.7333	0.7245	0.7409	0.4647	0.8218
H33x45	SMILES_extnd_connect_fps_2_1024	0.1	0.8178	0.8182	0.8079	0.8276	0.6356	0.8573
H33x45	SMILES_extnd_connect_fps_2_1024	0.15	0.7866	0.7872	0.7788	0.7945	0.5728	0.8465
H33x45	SMILES_extnd_connect_fps_2_1024	0.2	0.7603	0.7607	0.755	0.7655	0.5196	0.8375
H33x45	SMILES_extnd_connect_fps_2_1024	0.25	0.735	0.7355	0.7296	0.7405	0.4692	0.8294
H33x45	SMILES_extnd_connect_fps_2_1024	0.3	0.7452	0.7453	0.7426	0.7477	0.4894	0.8259
H33x45	SMILES_extnd_connect_fps_4_1024	0.1	0.8321	0.8324	0.8273	0.837	0.6639	0.8743
H33x45	SMILES_extnd_connect_fps_4_1024	0.15	0.798	0.7982	0.7957	0.8004	0.5954	0.8625
H33x45	SMILES_extnd_connect_fps_4_1024	0.2	0.7785	0.7784	0.7797	0.7772	0.5556	0.8529
H33x45	SMILES_extnd_connect_fps_4_1024	0.25	0.759	0.7588	0.7616	0.7564	0.5168	0.8454
H33x45	SMILES_extnd_connect_fps_4_1024	0.3	0.7743	0.7742	0.7751	0.7735	0.5474	0.8429
H33x45	selfies_4_hashed_1024	0.1	0.8115	0.8112	0.8143	0.8087	0.6201	0.8499
H33x45	selfies_4_hashed_1024	0.15	0.7783	0.7782	0.7788	0.7778	0.5549	0.8388
H33x45	selfies_4_hashed_1024	0.2	0.7548	0.7544	0.7588	0.7507	0.5081	0.8293
H33x45	selfies_4_hashed_1024	0.25	0.735	0.7346	0.7398	0.7302	0.4687	0.8205
H33x45	selfies_4_hashed_1024	0.3	0.7356	0.7354	0.7386	0.7327	0.4701	0.8155
H34x	core-substituent_fps	0.1	0.7484	0.7291	0.7697	0.7271	0.231	0.7869
H34x	core-substituent_fps	0.15	0.7335	0.7227	0.7454	0.7217	0.2086	0.7765
H34x	core-substituent_fps	0.2	0.7292	0.7102	0.75	0.7085	0.1995	0.7688
H34x	core-substituent_fps	0.25	0.7036	0.6926	0.7157	0.6916	0.1767	0.7622
H34x	core-substituent_fps	0.3	0.6831	0.6787	0.6878	0.6783	0.1588	0.7555
H34x	deepsmiles_4_hashed_1024	0.1	0.7864	0.7706	0.804	0.7688	0.2875	0.8447
H34x	deepsmiles_4_hashed_1024	0.15	0.7592	0.7481	0.7715	0.7469	0.2512	0.8265
H34x	deepsmiles_4_hashed_1024	0.2	0.7368	0.7271	0.7476	0.7261	0.2205	0.8143
H34x	deepsmiles_4_hashed_1024	0.25	0.7142	0.7028	0.7268	0.7016	0.1944	0.8037
H34x	deepsmiles_4_hashed_1024	0.3	0.7006	0.691	0.7113	0.69	0.1782	0.7951
H34x	morgan2_hashed_1024	0.1	0.8039	0.7898	0.8198	0.788	0.3223	0.8304
H34x	morgan2_hashed_1024	0.15	0.7604	0.7568	0.7645	0.7564	0.2586	0.8209
H34x	morgan2_hashed_1024	0.2	0.7367	0.7303	0.7438	0.7296	0.2235	0.8112
H34x	morgan2_hashed_1024	0.25	0.717	0.7149	0.7194	0.7146	0.1978	0.8023
H34x	morgan2_hashed_1024	0.3	0.7037	0.7048	0.7026	0.7049	0.1821	0.7951
H34x	morgan4_hashed_1024	0.1	0.7573	0.7454	0.7707	0.7439	0.2645	0.8107
H34x	morgan4_hashed_1024	0.15	0.7312	0.7224	0.7409	0.7214	0.2212	0.7976
H34x	morgan4_hashed_1024	0.2	0.7116	0.7091	0.7143	0.7089	0.194	0.7862
H34x	morgan4_hashed_1024	0.25	0.6814	0.6984	0.6627	0.7002	0.1635	0.7748
H34x	morgan4_hashed_1024	0.3	0.6586	0.6858	0.6286	0.6886	0.1411	0.7644

H34x	ngram_4_hashed_1024	0.1	0.8185	0.7786	0.8634	0.7736	0.3343	0.8566
H34x	ngram_4_hashed_1024	0.15	0.7823	0.7589	0.8085	0.7562	0.2796	0.8457
H34x	ngram_4_hashed_1024	0.2	0.7445	0.7415	0.7477	0.7412	0.2336	0.8345
H34x	ngram_4_hashed_1024	0.25	0.7173	0.7246	0.7092	0.7253	0.2006	0.8238
H34x	ngram_4_hashed_1024	0.3	0.7138	0.7238	0.7029	0.7248	0.195	0.8161
H34x	ngram_4_hashed_256	0.1	0.7964	0.7641	0.8333	0.7594	0.3235	0.8371
H34x	ngram_4_hashed_256	0.15	0.7678	0.7393	0.8	0.7357	0.2708	0.8276
H34x	ngram_4_hashed_256	0.2	0.7489	0.7154	0.7859	0.7118	0.2331	0.8203
H34x	ngram_4_hashed_256	0.25	0.7263	0.6985	0.757	0.6955	0.2062	0.8120
H34x	ngram_4_hashed_256	0.3	0.7155	0.6927	0.7406	0.6904	0.1918	0.8055
H34x	ngram_4_hashed_64	0.1	0.778	0.7429	0.8178	0.7382	0.289	0.8166
H34x	ngram_4_hashed_64	0.15	0.7547	0.7341	0.7778	0.7316	0.2553	0.8053
H34x	ngram_4_hashed_64	0.2	0.7262	0.7203	0.7327	0.7196	0.2137	0.7967
H34x	ngram_4_hashed_64	0.25	0.7072	0.7067	0.7079	0.7066	0.1893	0.7884
H34x	ngram_4_hashed_64	0.3	0.7015	0.7026	0.7003	0.7027	0.1802	0.7816
H34x	ngram_6_hashed_1024	0.1	0.8067	0.773	0.8447	0.7687	0.321	0.8492
H34x	ngram_6_hashed_1024	0.15	0.7767	0.7484	0.8083	0.7452	0.2695	0.8404
H34x	ngram_6_hashed_1024	0.2	0.738	0.7279	0.7492	0.7268	0.2227	0.8295
H34x	ngram_6_hashed_1024	0.25	0.7177	0.7074	0.7291	0.7063	0.1954	0.8195
H34x	ngram_6_hashed_1024	0.3	0.7	0.6979	0.7023	0.6977	0.1776	0.8100
H34x	ngram_6_hashed_256	0.1	0.8006	0.7798	0.8241	0.7772	0.3132	0.8301
H34x	ngram_6_hashed_256	0.15	0.7769	0.7582	0.7976	0.7563	0.2658	0.8247
H34x	ngram_6_hashed_256	0.2	0.7466	0.7342	0.7601	0.733	0.2264	0.8176
H34x	ngram_6_hashed_256	0.25	0.7297	0.7226	0.7376	0.7219	0.2065	0.8093
H34x	ngram_6_hashed_256	0.3	0.7138	0.7084	0.7197	0.7079	0.1895	0.8022
H34x	ngram_6_hashed_64	0.1	0.7401	0.7548	0.7236	0.7565	0.2401	0.7776
H34x	ngram_6_hashed_64	0.15	0.7221	0.7307	0.7126	0.7316	0.2093	0.7690
H34x	ngram_6_hashed_64	0.2	0.7033	0.7186	0.6865	0.7202	0.1877	0.7596
H34x	ngram_6_hashed_64	0.25	0.6794	0.7004	0.6562	0.7026	0.1619	0.7511
H34x	ngram_6_hashed_64	0.3	0.6645	0.6833	0.6438	0.6851	0.145	0.7440
H34x	ngramsPE_4_hashed_1024	0.1	0.8077	0.7727	0.8466	0.7689	0.3024	0.8583
H34x	ngramsPE_4_hashed_1024	0.15	0.7541	0.7489	0.7598	0.7483	0.2432	0.8398
H34x	ngramsPE_4_hashed_1024	0.2	0.7166	0.7241	0.7082	0.7249	0.2001	0.8235
H34x	ngramsPE_4_hashed_1024	0.25	0.6997	0.7086	0.6901	0.7094	0.1788	0.8097
H34x	ngramsPE_4_hashed_1024	0.3	0.6799	0.6935	0.6649	0.6948	0.1591	0.7984
H34x	SMILES_extnd_connect_fps_2_1024	0.1	0.8384	0.8196	0.8594	0.8174	0.3628	0.8834
H34x	SMILES_extnd_connect_fps_2_1024	0.15	0.8024	0.7928	0.8129	0.7918	0.3037	0.8736
H34x	SMILES_extnd_connect_fps_2_1024	0.2	0.7805	0.7753	0.7861	0.7748	0.2693	0.8648
H34x	SMILES_extnd_connect_fps_2_1024	0.25	0.7528	0.7518	0.754	0.7517	0.2348	0.8567
H34x	SMILES_extnd_connect_fps_2_1024	0.3	0.7645	0.7689	0.7597	0.7693	0.2521	0.8534
H34x	SMILES_extnd_connect_fps_4_1024	0.1	0.8208	0.8153	0.827	0.8147	0.3348	0.8609
H34x	SMILES_extnd_connect_fps_4_1024	0.15	0.7943	0.7841	0.8056	0.7831	0.2874	0.8519
H34x	SMILES_extnd_connect_fps_4_1024	0.2	0.7722	0.769	0.7758	0.7687	0.2577	0.8424
H34x	SMILES_extnd_connect_fps_4_1024	0.25	0.7478	0.7501	0.7453	0.7503	0.2286	0.8345
H34x	SMILES_extnd_connect_fps_4_1024	0.3	0.7602	0.7629	0.7571	0.7632	0.2418	0.8312
H34x	selfies_4_hashed_1024	0.1	0.7883	0.789	0.7874	0.7891	0.2954	0.8332
H34x	selfies_4_hashed_1024	0.15	0.7505	0.7518	0.749	0.752	0.2376	0.8204
H34x	selfies_4_hashed_1024	0.2	0.7254	0.7233	0.7276	0.7231	0.2044	0.8091
H34x	selfies_4_hashed_1024	0.25	0.7048	0.6989	0.7112	0.6983	0.1807	0.7985
H34x	selfies_4_hashed_1024	0.3	0.6859	0.6805	0.6919	0.68	0.1621	0.7886
H34x	consensus_cls_all	0.1	0.8881	0.8426	0.9394	0.8367	0.4452	NA
H34x	consensus_cls_all	0.15	0.824	0.8001	0.8505	0.7974	0.3367	NA
H34x	consensus_cls_all	0.2	0.7778	0.7618	0.7955	0.7602	0.2661	NA

H34x	consensus_cls_all	0.25	0.7561	0.7382	0.7758	0.7364	0.2335	NA
H34x	consensus_cls_all	0.3	0.7532	0.7392	0.7684	0.7379	0.2315	NA
H34x	consensus_pvals_all	0.1	0.8978	0.8622	0.9382	0.8573	0.4837	0.9375
H34x	consensus_pvals_all	0.15	0.8691	0.8386	0.9031	0.8352	0.4007	0.9274
H34x	consensus_pvals_all	0.2	0.8288	0.8109	0.8486	0.809	0.3332	0.9142
H34x	consensus_pvals_all	0.25	0.7978	0.7837	0.8134	0.7823	0.2898	0.9003
H34x	consensus_pvals_all	0.3	0.7648	0.7657	0.7638	0.7658	0.251	0.8885
H35x	core-substituent_fps	0.1	0.8212	0.8259	0.8147	0.8277	0.5103	0.8779
H35x	core-substituent_fps	0.15	0.79	0.7832	0.7994	0.7805	0.4407	0.8645
H35x	core-substituent_fps	0.2	0.7469	0.7528	0.7386	0.7553	0.376	0.8509
H35x	core-substituent_fps	0.25	0.7283	0.7268	0.7303	0.7262	0.343	0.8393
H35x	core-substituent_fps	0.3	0.7162	0.7127	0.7212	0.7112	0.325	0.8304
H35x	deepsmiles_4_hashed_1024	0.1	0.8112	0.825	0.7909	0.8315	0.5146	0.8735
H35x	deepsmiles_4_hashed_1024	0.15	0.7677	0.7788	0.7514	0.784	0.4273	0.8586
H35x	deepsmiles_4_hashed_1024	0.2	0.7471	0.7524	0.7395	0.7548	0.3832	0.8465
H35x	deepsmiles_4_hashed_1024	0.25	0.7226	0.7292	0.7131	0.7322	0.3434	0.8347
H35x	deepsmiles_4_hashed_1024	0.3	0.7148	0.7214	0.7053	0.7243	0.3293	0.8257
H35x	morgan2_hashed_1024	0.1	0.835	0.8264	0.848	0.822	0.5522	0.8810
H35x	morgan2_hashed_1024	0.15	0.8007	0.7923	0.8131	0.7882	0.4788	0.8704
H35x	morgan2_hashed_1024	0.2	0.766	0.764	0.7691	0.763	0.4189	0.8602
H35x	morgan2_hashed_1024	0.25	0.7399	0.7351	0.747	0.7329	0.3678	0.8515
H35x	morgan2_hashed_1024	0.3	0.7545	0.7535	0.7558	0.7531	0.3946	0.8478
H35x	morgan4_hashed_1024	0.1	0.8234	0.8107	0.843	0.8039	0.5313	0.8811
H35x	morgan4_hashed_1024	0.15	0.786	0.7727	0.8061	0.7659	0.4546	0.8668
H35x	morgan4_hashed_1024	0.2	0.7554	0.7475	0.7671	0.7438	0.3971	0.8532
H35x	morgan4_hashed_1024	0.25	0.7257	0.7251	0.7267	0.7247	0.3485	0.8410
H35x	morgan4_hashed_1024	0.3	0.7242	0.7278	0.719	0.7294	0.3445	0.8333
H35x	ngram_4_hashed_1024	0.1	0.8315	0.8274	0.838	0.8251	0.5604	0.8790
H35x	ngram_4_hashed_1024	0.15	0.7951	0.7944	0.7962	0.7941	0.4774	0.8672
H35x	ngram_4_hashed_1024	0.2	0.7738	0.7761	0.7706	0.7771	0.4286	0.8574
H35x	ngram_4_hashed_1024	0.25	0.7575	0.7626	0.75	0.7649	0.402	0.8506
H35x	ngram_4_hashed_1024	0.3	0.7749	0.7793	0.7686	0.7813	0.4342	0.8486
H35x	ngram_4_hashed_256	0.1	0.8236	0.8178	0.8323	0.815	0.5258	0.8762
H35x	ngram_4_hashed_256	0.15	0.787	0.788	0.7854	0.7886	0.4557	0.8625
H35x	ngram_4_hashed_256	0.2	0.7686	0.7658	0.7726	0.7645	0.4183	0.8518
H35x	ngram_4_hashed_256	0.25	0.748	0.7481	0.748	0.7481	0.3829	0.8429
H35x	ngram_4_hashed_256	0.3	0.7595	0.7612	0.757	0.7619	0.4032	0.8398
H35x	ngram_4_hashed_64	0.1	0.8243	0.8073	0.8511	0.7975	0.5369	0.8753
H35x	ngram_4_hashed_64	0.15	0.7944	0.7801	0.8157	0.7731	0.4654	0.8644
H35x	ngram_4_hashed_64	0.2	0.7671	0.7559	0.7837	0.7506	0.4167	0.8538
H35x	ngram_4_hashed_64	0.25	0.7441	0.7318	0.762	0.7262	0.3718	0.8439
H35x	ngram_4_hashed_64	0.3	0.7411	0.7299	0.7573	0.7249	0.3648	0.8377
H35x	ngram_6_hashed_1024	0.1	0.821	0.8347	0.8	0.8419	0.5463	0.8577
H35x	ngram_6_hashed_1024	0.15	0.7787	0.7961	0.7525	0.8049	0.4588	0.8476
H35x	ngram_6_hashed_1024	0.2	0.7539	0.7657	0.7363	0.7716	0.4066	0.8381
H35x	ngram_6_hashed_1024	0.25	0.7319	0.7403	0.7195	0.7442	0.3593	0.8292
H35x	ngram_6_hashed_1024	0.3	0.7409	0.7489	0.7293	0.7525	0.375	0.8245
H35x	ngram_6_hashed_256	0.1	0.8275	0.8182	0.8418	0.8132	0.5407	0.8758
H35x	ngram_6_hashed_256	0.15	0.7907	0.7892	0.7931	0.7884	0.4664	0.8622
H35x	ngram_6_hashed_256	0.2	0.7691	0.7665	0.7729	0.7653	0.4216	0.8510
H35x	ngram_6_hashed_256	0.25	0.7395	0.7369	0.7433	0.7358	0.3673	0.8412
H35x	ngram_6_hashed_256	0.3	0.7443	0.7414	0.7484	0.7401	0.3734	0.8359
H35x	ngram_6_hashed_64	0.1	0.8058	0.8039	0.8087	0.8029	0.4983	0.8507

H35x	ngram_6_hashed_64	0.15	0.7747	0.778	0.7697	0.7796	0.4357	0.8387
H35x	ngram_6_hashed_64	0.2	0.7395	0.7557	0.716	0.763	0.3749	0.8267
H35x	ngram_6_hashed_64	0.25	0.7173	0.7339	0.6931	0.7415	0.3365	0.8164
H35x	ngram_6_hashed_64	0.3	0.7039	0.7176	0.6841	0.7238	0.3128	0.8084
H35x	ngramsPE_4_hashed_1024	0.1	0.8075	0.8025	0.8148	0.8001	0.4957	0.8574
H35x	ngramsPE_4_hashed_1024	0.15	0.7676	0.7637	0.7733	0.7619	0.419	0.8430
H35x	ngramsPE_4_hashed_1024	0.2	0.7392	0.7395	0.7389	0.7396	0.3709	0.8303
H35x	ngramsPE_4_hashed_1024	0.25	0.7261	0.7182	0.7374	0.7147	0.3427	0.8191
H35x	ngramsPE_4_hashed_1024	0.3	0.7161	0.7074	0.7288	0.7035	0.3242	0.8106
H35x	SMILES_extnd_connect_fps_2_1024	0.1	0.8036	0.8138	0.788	0.8191	0.5061	0.8613
H35x	SMILES_extnd_connect_fps_2_1024	0.15	0.7788	0.7831	0.7725	0.7852	0.4445	0.8481
H35x	SMILES_extnd_connect_fps_2_1024	0.2	0.7475	0.7542	0.7377	0.7573	0.3894	0.8369
H35x	SMILES_extnd_connect_fps_2_1024	0.25	0.728	0.7323	0.7216	0.7343	0.3499	0.8274
H35x	SMILES_extnd_connect_fps_2_1024	0.3	0.7339	0.7328	0.7354	0.7323	0.3585	0.8224
H35x	SMILES_extnd_connect_fps_4_1024	0.1	0.841	0.8444	0.8359	0.846	0.5668	0.8871
H35x	SMILES_extnd_connect_fps_4_1024	0.15	0.8025	0.8043	0.8	0.805	0.4854	0.8775
H35x	SMILES_extnd_connect_fps_4_1024	0.2	0.7758	0.7732	0.7795	0.772	0.4316	0.8678
H35x	SMILES_extnd_connect_fps_4_1024	0.25	0.7537	0.7555	0.751	0.7563	0.3946	0.8591
H35x	SMILES_extnd_connect_fps_4_1024	0.3	0.7573	0.7563	0.7588	0.7558	0.3991	0.8542
H35x	selfies_4_hashed_1024	0.1	0.7916	0.792	0.7909	0.7923	0.4717	0.8647
H35x	selfies_4_hashed_1024	0.15	0.7696	0.7596	0.7839	0.7552	0.4133	0.8503
H35x	selfies_4_hashed_1024	0.2	0.739	0.7397	0.738	0.74	0.3643	0.8355
H35x	selfies_4_hashed_1024	0.25	0.7158	0.7101	0.7241	0.7076	0.3235	0.8219
H35x	selfies_4_hashed_1024	0.3	0.7015	0.6906	0.7172	0.6857	0.3005	0.8103
H35x	consensus_cls_all	0.1	0.8805	0.869	0.898	0.8629	0.6494	NA
H35x	consensus_cls_all	0.15	0.8232	0.8187	0.8301	0.8164	0.5317	NA
H35x	consensus_cls_all	0.2	0.7867	0.7754	0.8033	0.7702	0.4482	NA
H35x	consensus_cls_all	0.25	0.7749	0.7605	0.7957	0.7541	0.4232	NA
H35x	consensus_cls_all	0.3	0.7745	0.7597	0.7961	0.753	0.4224	NA
H35x	consensus_pvals_all	0.1	0.8995	0.89	0.9139	0.8852	0.6914	0.9429
H35x	consensus_pvals_all	0.15	0.8613	0.8498	0.8783	0.8442	0.5986	0.9300
H35x	consensus_pvals_all	0.2	0.8219	0.8173	0.8286	0.8151	0.5243	0.9165
H35x	consensus_pvals_all	0.25	0.7957	0.7866	0.8088	0.7826	0.4639	0.9045
H35x	consensus_pvals_all	0.3	0.7849	0.7791	0.7935	0.7764	0.4477	0.8968
H36x01	consensus_cls_all	0.1	0.8745	0.8633	0.8929	0.8561	0.6559	NA
H36x01	consensus_cls_all	0.15	0.8245	0.8207	0.8304	0.8186	0.54	NA
H36x01	consensus_cls_all	0.2	0.7814	0.7711	0.7966	0.7662	0.4418	NA
H36x01	consensus_cls_all	0.25	0.7589	0.7528	0.7678	0.7501	0.3993	NA
H36x01	consensus_cls_all	0.3	0.7569	0.7536	0.7616	0.7521	0.3967	NA
H36x01	consensus_pvals_all	0.1	0.8918	0.8811	0.9099	0.8737	0.6977	0.9321
H36x01	consensus_pvals_all	0.15	0.8552	0.8505	0.8626	0.8479	0.606	0.9185
H36x01	consensus_pvals_all	0.2	0.8157	0.8172	0.8134	0.818	0.5221	0.9052
H36x01	consensus_pvals_all	0.25	0.785	0.7846	0.7857	0.7844	0.4521	0.8925
H36x01	consensus_pvals_all	0.3	0.7647	0.7707	0.756	0.7735	0.4167	0.8826
H36x01	core-substituent_fps	0.1	0.8073	0.7952	0.8261	0.7885	0.5038	0.8469
H36x01	core-substituent_fps	0.15	0.775	0.7691	0.7836	0.7663	0.4316	0.8362
H36x01	core-substituent_fps	0.2	0.747	0.7479	0.7457	0.7483	0.3821	0.8254
H36x01	core-substituent_fps	0.25	0.7211	0.7285	0.7102	0.7319	0.3399	0.8150
H36x01	core-substituent_fps	0.3	0.7094	0.7134	0.7036	0.7152	0.3179	0.8068
H36x01	deepsmiles_4_hashed_1024	0.1	0.8099	0.8053	0.8171	0.8027	0.517	0.8500
H36x01	deepsmiles_4_hashed_1024	0.15	0.7739	0.7724	0.7762	0.7717	0.4412	0.8395
H36x01	deepsmiles_4_hashed_1024	0.2	0.7476	0.7436	0.7534	0.7417	0.3859	0.8289
H36x01	deepsmiles_4_hashed_1024	0.25	0.7182	0.7155	0.7222	0.7143	0.3323	0.8185

H36x01	deepsmls_4_hashed_1024	0.3	0.7121	0.7141	0.7092	0.715	0.3232	0.8110
H36x01	morgan2_hashed_1024	0.1	0.8307	0.8077	0.8673	0.7941	0.5473	0.8929
H36x01	morgan2_hashed_1024	0.15	0.7966	0.7836	0.8163	0.777	0.4754	0.8785
H36x01	morgan2_hashed_1024	0.2	0.7676	0.7646	0.772	0.7632	0.4222	0.8646
H36x01	morgan2_hashed_1024	0.25	0.7486	0.7432	0.7564	0.7407	0.3822	0.8540
H36x01	morgan2_hashed_1024	0.3	0.7482	0.7483	0.7479	0.7484	0.3836	0.8481
H36x01	morgan4_hashed_1024	0.1	0.8174	0.7941	0.8553	0.7795	0.5278	0.8816
H36x01	morgan4_hashed_1024	0.15	0.788	0.7682	0.818	0.7579	0.4585	0.8674
H36x01	morgan4_hashed_1024	0.2	0.7545	0.7457	0.7677	0.7414	0.3974	0.8541
H36x01	morgan4_hashed_1024	0.25	0.7349	0.7287	0.7439	0.7259	0.358	0.8422
H36x01	morgan4_hashed_1024	0.3	0.7224	0.7191	0.7271	0.7177	0.3378	0.8333
H36x01	ngram_4_hashed_1024	0.1	0.8302	0.8028	0.8765	0.7839	0.5571	0.8799
H36x01	ngram_4_hashed_1024	0.15	0.7918	0.7742	0.8196	0.7639	0.4768	0.8690
H36x01	ngram_4_hashed_1024	0.2	0.7643	0.7531	0.781	0.7475	0.4174	0.8583
H36x01	ngram_4_hashed_1024	0.25	0.7359	0.7315	0.7425	0.7293	0.3637	0.8474
H36x01	ngram_4_hashed_1024	0.3	0.7368	0.7391	0.7336	0.7401	0.3674	0.8409
H36x01	ngram_4_hashed_256	0.1	0.8054	0.788	0.8339	0.7768	0.5108	0.8652
H36x01	ngram_4_hashed_256	0.15	0.7767	0.7643	0.7962	0.7573	0.4478	0.8510
H36x01	ngram_4_hashed_256	0.2	0.7518	0.7393	0.7708	0.7328	0.3957	0.8398
H36x01	ngram_4_hashed_256	0.25	0.7332	0.7294	0.7389	0.7276	0.3588	0.8291
H36x01	ngram_4_hashed_256	0.3	0.7271	0.7251	0.7301	0.7241	0.3473	0.8220
H36x01	ngram_4_hashed_64	0.1	0.8083	0.8022	0.818	0.7986	0.5176	0.8561
H36x01	ngram_4_hashed_64	0.15	0.7649	0.7667	0.7621	0.7677	0.4281	0.8421
H36x01	ngram_4_hashed_64	0.2	0.7423	0.7464	0.7363	0.7483	0.3808	0.8295
H36x01	ngram_4_hashed_64	0.25	0.7199	0.7255	0.7118	0.728	0.3382	0.8182
H36x01	ngram_4_hashed_64	0.3	0.7024	0.7135	0.6864	0.7185	0.3091	0.8090
H36x01	ngram_6_hashed_1024	0.1	0.8194	0.8069	0.8399	0.7988	0.5404	0.8641
H36x01	ngram_6_hashed_1024	0.15	0.7871	0.775	0.8057	0.7685	0.4636	0.8555
H36x01	ngram_6_hashed_1024	0.2	0.7592	0.7477	0.7762	0.7422	0.404	0.8457
H36x01	ngram_6_hashed_1024	0.25	0.7358	0.7322	0.7411	0.7305	0.3632	0.8361
H36x01	ngram_6_hashed_1024	0.3	0.7234	0.7255	0.7203	0.7265	0.3424	0.8288
H36x01	ngram_6_hashed_256	0.1	0.8017	0.7931	0.8157	0.7877	0.5075	0.8547
H36x01	ngram_6_hashed_256	0.15	0.7706	0.7579	0.7902	0.7511	0.4325	0.8431
H36x01	ngram_6_hashed_256	0.2	0.7449	0.7383	0.7547	0.7351	0.3824	0.8321
H36x01	ngram_6_hashed_256	0.25	0.7286	0.7266	0.7314	0.7257	0.35	0.8219
H36x01	ngram_6_hashed_256	0.3	0.7171	0.7198	0.7133	0.7209	0.3314	0.8142
H36x01	ngram_6_hashed_64	0.1	0.7954	0.7861	0.8105	0.7803	0.4946	0.8401
H36x01	ngram_6_hashed_64	0.15	0.7728	0.7607	0.7915	0.754	0.4386	0.8298
H36x01	ngram_6_hashed_64	0.2	0.7438	0.7391	0.751	0.7366	0.3836	0.8200
H36x01	ngram_6_hashed_64	0.25	0.7162	0.7155	0.7173	0.7152	0.3324	0.8102
H36x01	ngram_6_hashed_64	0.3	0.6994	0.6993	0.6995	0.6992	0.3015	0.8017
H36x01	ngramsPE_4_hashed_1024	0.1	0.815	0.8026	0.8349	0.7952	0.5252	0.8632
H36x01	ngramsPE_4_hashed_1024	0.15	0.7795	0.767	0.7984	0.7606	0.444	0.8520
H36x01	ngramsPE_4_hashed_1024	0.2	0.7506	0.7412	0.7647	0.7365	0.39	0.8409
H36x01	ngramsPE_4_hashed_1024	0.25	0.7303	0.7222	0.7421	0.7184	0.3517	0.8301
H36x01	ngramsPE_4_hashed_1024	0.3	0.7175	0.7137	0.723	0.712	0.33	0.8214
H36x01	SMILES_extnd_connect_fps_2_1024	0.1	0.8143	0.8028	0.8327	0.7959	0.5259	0.8740
H36x01	SMILES_extnd_connect_fps_2_1024	0.15	0.7935	0.7801	0.8137	0.7733	0.4679	0.8615
H36x01	SMILES_extnd_connect_fps_2_1024	0.2	0.7655	0.7572	0.7776	0.7534	0.4118	0.8503
H36x01	SMILES_extnd_connect_fps_2_1024	0.25	0.7374	0.7344	0.7416	0.7331	0.3629	0.8400
H36x01	SMILES_extnd_connect_fps_2_1024	0.3	0.7269	0.724	0.7311	0.7227	0.346	0.8327
H36x01	SMILES_extnd_connect_fps_4_1024	0.1	0.8265	0.8211	0.8346	0.8184	0.5378	0.8798
H36x01	SMILES_extnd_connect_fps_4_1024	0.15	0.7852	0.7838	0.7872	0.7832	0.4548	0.8652

H36x01	SMILES_extnd_connect_fps_4_1024	0.2	0.7575	0.7594	0.7546	0.7603	0.4015	0.8535
H36x01	SMILES_extnd_connect_fps_4_1024	0.25	0.7373	0.7356	0.7399	0.7348	0.3637	0.8435
H36x01	SMILES_extnd_connect_fps_4_1024	0.3	0.7307	0.7309	0.7304	0.731	0.3533	0.8367
H36x01	selfies_4_hashed_1024	0.1	0.8047	0.7858	0.8347	0.7747	0.4995	0.8523
H36x01	selfies_4_hashed_1024	0.15	0.7678	0.7641	0.7734	0.7622	0.4252	0.8403
H36x01	selfies_4_hashed_1024	0.2	0.7346	0.7345	0.7348	0.7345	0.3631	0.8288
H36x01	selfies_4_hashed_1024	0.25	0.7142	0.7125	0.7166	0.7117	0.3264	0.8176
H36x01	selfies_4_hashed_1024	0.3	0.6988	0.6968	0.7017	0.6959	0.2984	0.8080
H40x	consensus_cls_all	0.1	0.8498	0.8491	0.8508	0.8487	0.6118	NA
H40x	consensus_cls_all	0.15	0.8167	0.8122	0.8241	0.8094	0.5372	NA
H40x	consensus_cls_all	0.2	0.7752	0.7688	0.7855	0.7649	0.4533	NA
H40x	consensus_cls_all	0.25	0.7489	0.7397	0.7637	0.7341	0.4048	NA
H40x	consensus_cls_all	0.3	0.748	0.7358	0.7674	0.7285	0.402	NA
H40x	consensus_pvals_all	0.1	0.8665	0.865	0.8689	0.864	0.6443	0.9050
H40x	consensus_pvals_all	0.15	0.8397	0.8368	0.8443	0.8351	0.584	0.8917
H40x	consensus_pvals_all	0.2	0.8104	0.8065	0.8165	0.8042	0.5205	0.8806
H40x	consensus_pvals_all	0.25	0.773	0.7696	0.7784	0.7676	0.4507	0.8700
H40x	consensus_pvals_all	0.3	0.7496	0.7479	0.7522	0.7469	0.4089	0.8603
H40x	core-substituent_fps	0.1	0.7756	0.7793	0.7697	0.7816	0.4643	0.8108
H40x	core-substituent_fps	0.15	0.7465	0.7527	0.7366	0.7565	0.4078	0.7997
H40x	core-substituent_fps	0.2	0.7197	0.7284	0.7057	0.7336	0.3592	0.7896
H40x	core-substituent_fps	0.25	0.6988	0.706	0.6874	0.7102	0.3218	0.7806
H40x	core-substituent_fps	0.3	0.6795	0.6866	0.6683	0.6908	0.2887	0.7724
H40x	deepsmiles_4_hashed_1024	0.1	0.7964	0.7982	0.7935	0.7993	0.5034	0.8307
H40x	deepsmiles_4_hashed_1024	0.15	0.7603	0.7647	0.7532	0.7674	0.4356	0.8196
H40x	deepsmiles_4_hashed_1024	0.2	0.7362	0.7426	0.726	0.7464	0.3894	0.8091
H40x	deepsmiles_4_hashed_1024	0.25	0.7141	0.7184	0.7072	0.7209	0.3486	0.7998
H40x	deepsmiles_4_hashed_1024	0.3	0.6979	0.7004	0.694	0.7019	0.3197	0.7918
H40x	morgan2_hashed_1024	0.1	0.818	0.8162	0.821	0.815	0.5476	0.8624
H40x	morgan2_hashed_1024	0.15	0.7885	0.7846	0.7948	0.7822	0.4833	0.8509
H40x	morgan2_hashed_1024	0.2	0.7629	0.76	0.7675	0.7583	0.4343	0.8404
H40x	morgan2_hashed_1024	0.25	0.7374	0.7373	0.7374	0.7373	0.3889	0.8309
H40x	morgan2_hashed_1024	0.3	0.7356	0.7384	0.7312	0.74	0.3866	0.8249
H40x	morgan4_hashed_1024	0.1	0.811	0.8077	0.8163	0.8057	0.5246	0.8608
H40x	morgan4_hashed_1024	0.15	0.773	0.7682	0.7805	0.7654	0.4493	0.8465
H40x	morgan4_hashed_1024	0.2	0.7437	0.7452	0.7414	0.7461	0.3988	0.8331
H40x	morgan4_hashed_1024	0.25	0.7231	0.7237	0.7222	0.724	0.3613	0.8216
H40x	morgan4_hashed_1024	0.3	0.7046	0.705	0.7039	0.7052	0.3297	0.8117
H40x	ngram_4_hashed_1024	0.1	0.8152	0.8178	0.8111	0.8193	0.539	0.8520
H40x	ngram_4_hashed_1024	0.15	0.7905	0.7892	0.7925	0.7885	0.4842	0.8421
H40x	ngram_4_hashed_1024	0.2	0.7655	0.7638	0.7683	0.7627	0.4357	0.8335
H40x	ngram_4_hashed_1024	0.25	0.7371	0.737	0.7373	0.737	0.3866	0.8254
H40x	ngram_4_hashed_1024	0.3	0.7328	0.7353	0.7288	0.7367	0.3803	0.8201
H40x	ngram_4_hashed_256	0.1	0.8128	0.8125	0.8133	0.8123	0.5346	0.8445
H40x	ngram_4_hashed_256	0.15	0.7824	0.7819	0.7832	0.7816	0.4703	0.8349
H40x	ngram_4_hashed_256	0.2	0.7506	0.7502	0.7512	0.75	0.4117	0.8259
H40x	ngram_4_hashed_256	0.25	0.7311	0.7306	0.732	0.7303	0.3753	0.8176
H40x	ngram_4_hashed_256	0.3	0.7197	0.7197	0.7196	0.7197	0.3561	0.8109
H40x	ngram_4_hashed_64	0.1	0.8049	0.7968	0.8182	0.7916	0.5148	0.8396
H40x	ngram_4_hashed_64	0.15	0.7776	0.7726	0.7857	0.7696	0.4613	0.8294
H40x	ngram_4_hashed_64	0.2	0.7501	0.7462	0.7564	0.7439	0.4093	0.8200
H40x	ngram_4_hashed_64	0.25	0.7228	0.7198	0.7276	0.7181	0.3601	0.8111
H40x	ngram_4_hashed_64	0.3	0.7056	0.7015	0.7122	0.699	0.3306	0.8035

H40x	ngram_6_hashed_1024	0.1	0.804	0.8052	0.8019	0.806	0.5158	0.8409
H40x	ngram_6_hashed_1024	0.15	0.7764	0.7796	0.7711	0.7817	0.465	0.8306
H40x	ngram_6_hashed_1024	0.2	0.7547	0.7589	0.7479	0.7614	0.4218	0.8214
H40x	ngram_6_hashed_1024	0.25	0.7273	0.7341	0.7165	0.7382	0.3726	0.8130
H40x	ngram_6_hashed_1024	0.3	0.7174	0.7242	0.7065	0.7284	0.3553	0.8068
H40x	ngram_6_hashed_256	0.1	0.8011	0.7985	0.8053	0.797	0.507	0.8344
H40x	ngram_6_hashed_256	0.15	0.775	0.7714	0.7808	0.7692	0.4569	0.8243
H40x	ngram_6_hashed_256	0.2	0.7439	0.7455	0.7414	0.7464	0.4007	0.8150
H40x	ngram_6_hashed_256	0.25	0.7186	0.7208	0.7149	0.7222	0.3559	0.8064
H40x	ngram_6_hashed_256	0.3	0.6987	0.7011	0.6948	0.7026	0.3208	0.7981
H40x	ngram_6_hashed_64	0.1	0.7954	0.7915	0.802	0.7889	0.5018	0.8212
H40x	ngram_6_hashed_64	0.15	0.7625	0.7593	0.7676	0.7573	0.4366	0.8129
H40x	ngram_6_hashed_64	0.2	0.7338	0.7342	0.7331	0.7344	0.3832	0.8042
H40x	ngram_6_hashed_64	0.25	0.7142	0.7136	0.7151	0.7132	0.3474	0.7959
H40x	ngram_6_hashed_64	0.3	0.6983	0.6951	0.7035	0.6931	0.319	0.7881
H40x	ngramsPE_4_hashed_1024	0.1	0.7941	0.796	0.7909	0.7972	0.4981	0.8411
H40x	ngramsPE_4_hashed_1024	0.15	0.7724	0.7727	0.772	0.7728	0.452	0.8283
H40x	ngramsPE_4_hashed_1024	0.2	0.7404	0.7426	0.7368	0.744	0.3931	0.8176
H40x	ngramsPE_4_hashed_1024	0.25	0.7173	0.7175	0.717	0.7176	0.3524	0.8080
H40x	ngramsPE_4_hashed_1024	0.3	0.6975	0.6968	0.6986	0.6964	0.3171	0.7993
H40x	SMILES_extnd_connect_fps_2_1024	0.1	0.7926	0.7911	0.7949	0.7902	0.4944	0.8213
H40x	SMILES_extnd_connect_fps_2_1024	0.15	0.7624	0.761	0.7647	0.7601	0.4321	0.8118
H40x	SMILES_extnd_connect_fps_2_1024	0.2	0.7392	0.7387	0.7401	0.7384	0.3884	0.8032
H40x	SMILES_extnd_connect_fps_2_1024	0.25	0.7156	0.7161	0.7148	0.7164	0.3495	0.7949
H40x	SMILES_extnd_connect_fps_2_1024	0.3	0.6947	0.6965	0.6918	0.6976	0.3136	0.7873
H40x	SMILES_extnd_connect_fps_4_1024	0.1	0.8067	0.8006	0.8166	0.7968	0.5162	0.8439
H40x	SMILES_extnd_connect_fps_4_1024	0.15	0.7697	0.7682	0.7722	0.7673	0.4481	0.8324
H40x	SMILES_extnd_connect_fps_4_1024	0.2	0.7413	0.7402	0.7432	0.7395	0.394	0.8221
H40x	SMILES_extnd_connect_fps_4_1024	0.25	0.7119	0.7153	0.7066	0.7172	0.3441	0.8118
H40x	SMILES_extnd_connect_fps_4_1024	0.3	0.6989	0.7003	0.6965	0.7012	0.3203	0.8033
H40x	selfies_4_hashed_1024	0.1	0.7848	0.7797	0.7929	0.7767	0.4724	0.8379
H40x	selfies_4_hashed_1024	0.15	0.7585	0.7551	0.7637	0.7532	0.4193	0.8247
H40x	selfies_4_hashed_1024	0.2	0.7384	0.7372	0.7404	0.7364	0.3859	0.8126
H40x	selfies_4_hashed_1024	0.25	0.7147	0.7123	0.7184	0.7109	0.3462	0.8020
H40x	selfies_4_hashed_1024	0.3	0.6948	0.6926	0.6982	0.6913	0.3126	0.7924
H41x	consensus_cls_all	0.1	0.8514	0.8518	0.8456	0.8572	0.7024	NA
H41x	consensus_cls_all	0.15	0.8074	0.8075	0.8025	0.8123	0.6146	NA
H41x	consensus_cls_all	0.2	0.7697	0.7697	0.7704	0.7691	0.5394	NA
H41x	consensus_cls_all	0.25	0.7478	0.7476	0.7572	0.7384	0.4956	NA
H41x	consensus_cls_all	0.3	0.7446	0.7443	0.7588	0.7303	0.4891	NA
H41x	consensus_pvals_all	0.1	0.8596	0.86	0.8549	0.8643	0.7185	0.8941
H41x	consensus_pvals_all	0.15	0.8278	0.828	0.8227	0.8329	0.6554	0.8815
H41x	consensus_pvals_all	0.2	0.7952	0.7953	0.7907	0.7996	0.5902	0.8700
H41x	consensus_pvals_all	0.25	0.7659	0.7658	0.7674	0.7643	0.5316	0.8597
H41x	consensus_pvals_all	0.3	0.7494	0.7493	0.7522	0.7466	0.4987	0.8514
H41x	core-substituent_fps	0.1	0.778	0.7779	0.7812	0.7748	0.5559	0.8133
H41x	core-substituent_fps	0.15	0.7499	0.7498	0.7528	0.7469	0.4996	0.8014
H41x	core-substituent_fps	0.2	0.7242	0.7241	0.7328	0.7156	0.4483	0.7908
H41x	core-substituent_fps	0.25	0.7109	0.7107	0.7207	0.7011	0.4217	0.7813
H41x	core-substituent_fps	0.3	0.689	0.6888	0.7004	0.6777	0.378	0.7728
H41x	deepsmiles_4_hashed_1024	0.1	0.8114	0.8114	0.8117	0.811	0.6222	0.8426
H41x	deepsmiles_4_hashed_1024	0.15	0.7787	0.7787	0.777	0.7803	0.5572	0.8330
H41x	deepsmiles_4_hashed_1024	0.2	0.7513	0.7512	0.7546	0.7479	0.5024	0.8236

H41x	deepsmiles_4_hashed_1024	0.25	0.7287	0.7286	0.732	0.7253	0.4572	0.8145
H41x	deepsmiles_4_hashed_1024	0.3	0.7143	0.7141	0.7214	0.7071	0.4285	0.8072
H41x	morgan2_hashed_1024	0.1	0.8278	0.828	0.8227	0.8329	0.6555	0.8643
H41x	morgan2_hashed_1024	0.15	0.7932	0.7932	0.7915	0.7948	0.5863	0.8543
H41x	morgan2_hashed_1024	0.2	0.7655	0.7655	0.764	0.767	0.531	0.8445
H41x	morgan2_hashed_1024	0.25	0.7401	0.7401	0.7427	0.7375	0.4801	0.8352
H41x	morgan2_hashed_1024	0.3	0.7429	0.7429	0.7421	0.7437	0.4858	0.8300
H41x	morgan4_hashed_1024	0.1	0.8138	0.8142	0.805	0.8227	0.6277	0.8497
H41x	morgan4_hashed_1024	0.15	0.7856	0.7855	0.7878	0.7834	0.5709	0.8396
H41x	morgan4_hashed_1024	0.2	0.7589	0.7589	0.7602	0.7576	0.5177	0.8306
H41x	morgan4_hashed_1024	0.25	0.7355	0.7354	0.7362	0.7347	0.4708	0.8222
H41x	morgan4_hashed_1024	0.3	0.7328	0.7327	0.7362	0.7293	0.4654	0.8169
H41x	ngram_4_hashed_1024	0.1	0.812	0.8129	0.7984	0.8257	0.6242	0.8467
H41x	ngram_4_hashed_1024	0.15	0.782	0.7823	0.7746	0.7895	0.5641	0.8366
H41x	ngram_4_hashed_1024	0.2	0.7557	0.756	0.7491	0.7623	0.5114	0.8271
H41x	ngram_4_hashed_1024	0.25	0.7343	0.7343	0.7333	0.7353	0.4685	0.8184
H41x	ngram_4_hashed_1024	0.3	0.7269	0.7268	0.7296	0.7241	0.4537	0.8123
H41x	ngram_4_hashed_256	0.1	0.8154	0.8162	0.8048	0.826	0.6304	0.8484
H41x	ngram_4_hashed_256	0.15	0.7852	0.7857	0.7762	0.7942	0.5701	0.8385
H41x	ngram_4_hashed_256	0.2	0.7586	0.7589	0.7517	0.7655	0.5171	0.8291
H41x	ngram_4_hashed_256	0.25	0.7329	0.7331	0.7237	0.7421	0.4658	0.8204
H41x	ngram_4_hashed_256	0.3	0.7242	0.7243	0.7197	0.7287	0.4484	0.8138
H41x	ngram_4_hashed_64	0.1	0.812	0.8125	0.8038	0.8203	0.6238	0.8420
H41x	ngram_4_hashed_64	0.15	0.7747	0.7752	0.7652	0.7842	0.5494	0.8320
H41x	ngram_4_hashed_64	0.2	0.7487	0.7488	0.7443	0.753	0.4972	0.8223
H41x	ngram_4_hashed_64	0.25	0.7281	0.7281	0.7273	0.7289	0.4561	0.8130
H41x	ngram_4_hashed_64	0.3	0.7131	0.7132	0.7119	0.7143	0.4262	0.8054
H41x	ngram_6_hashed_1024	0.1	0.8092	0.8095	0.8047	0.8136	0.6175	0.8434
H41x	ngram_6_hashed_1024	0.15	0.781	0.7813	0.7755	0.7865	0.5618	0.8328
H41x	ngram_6_hashed_1024	0.2	0.7535	0.7536	0.7514	0.7557	0.5068	0.8232
H41x	ngram_6_hashed_1024	0.25	0.728	0.728	0.7286	0.7273	0.4558	0.8141
H41x	ngram_6_hashed_1024	0.3	0.7206	0.7205	0.7246	0.7166	0.4411	0.8079
H41x	ngram_6_hashed_256	0.1	0.8054	0.8056	0.8021	0.8086	0.61	0.8342
H41x	ngram_6_hashed_256	0.15	0.7746	0.7748	0.7703	0.779	0.549	0.8241
H41x	ngram_6_hashed_256	0.2	0.755	0.7549	0.7564	0.7535	0.5097	0.8154
H41x	ngram_6_hashed_256	0.25	0.731	0.731	0.7316	0.7305	0.462	0.8072
H41x	ngram_6_hashed_256	0.3	0.7183	0.7183	0.7213	0.7154	0.4366	0.8006
H41x	ngram_6_hashed_64	0.1	0.8014	0.8016	0.7988	0.804	0.6019	0.8278
H41x	ngram_6_hashed_64	0.15	0.7704	0.7702	0.7748	0.7659	0.5401	0.8189
H41x	ngram_6_hashed_64	0.2	0.7461	0.7461	0.7462	0.7461	0.492	0.8103
H41x	ngram_6_hashed_64	0.25	0.7173	0.7174	0.716	0.7186	0.4345	0.8017
H41x	ngram_6_hashed_64	0.3	0.6994	0.6994	0.6956	0.7031	0.3987	0.7941
H41x	ngramsPE_4_hashed_1024	0.1	0.807	0.8075	0.7976	0.8163	0.6138	0.8442
H41x	ngramsPE_4_hashed_1024	0.15	0.7744	0.7746	0.7706	0.7783	0.5487	0.8333
H41x	ngramsPE_4_hashed_1024	0.2	0.7502	0.7504	0.744	0.7565	0.5004	0.8229
H41x	ngramsPE_4_hashed_1024	0.25	0.726	0.7263	0.7169	0.7351	0.452	0.8134
H41x	ngramsPE_4_hashed_1024	0.3	0.7129	0.713	0.7057	0.7201	0.4258	0.8060
H41x	SMILES_extnd_connect_fps_2_1024	0.1	0.8005	0.8003	0.8033	0.7977	0.6005	0.8296
H41x	SMILES_extnd_connect_fps_2_1024	0.15	0.7672	0.7672	0.767	0.7674	0.5342	0.8194
H41x	SMILES_extnd_connect_fps_2_1024	0.2	0.7406	0.7405	0.7419	0.7392	0.481	0.8092
H41x	SMILES_extnd_connect_fps_2_1024	0.25	0.7183	0.7183	0.7198	0.7169	0.4366	0.8000
H41x	SMILES_extnd_connect_fps_2_1024	0.3	0.7016	0.7015	0.7066	0.6967	0.4031	0.7922
H41x	SMILES_extnd_connect_fps_4_1024	0.1	0.8074	0.8075	0.8047	0.8102	0.6147	0.8438

H41x	SMILES_extnd_connect_fps_4_1024	0.15	0.7772	0.7772	0.7774	0.7769	0.5542	0.8322
H41x	SMILES_extnd_connect_fps_4_1024	0.2	0.7512	0.7512	0.7531	0.7493	0.5023	0.8222
H41x	SMILES_extnd_connect_fps_4_1024	0.25	0.7254	0.7254	0.7255	0.7253	0.4508	0.8127
H41x	SMILES_extnd_connect_fps_4_1024	0.3	0.7109	0.7109	0.712	0.7097	0.4217	0.8051
H41x	selfies_4_hashed_1024	0.1	0.7995	0.7996	0.7962	0.8028	0.5988	0.8348
H41x	selfies_4_hashed_1024	0.15	0.7693	0.7694	0.7645	0.7742	0.5386	0.8239
H41x	selfies_4_hashed_1024	0.2	0.7494	0.7495	0.7443	0.7545	0.4987	0.8141
H41x	selfies_4_hashed_1024	0.25	0.7274	0.7275	0.7246	0.7302	0.4548	0.8054
H41x	selfies_4_hashed_1024	0.3	0.7112	0.7113	0.7093	0.7132	0.4224	0.7981

a. ROC_auc not available (NA) since consensus assignments were performed on classes and not p-value differences (p_value_H-statement_class – p_value_non-H-statement_class).