Supplementary Information for

Gibbs-Helmholtz Graph Neural Network: capturing the temperature dependency of infinite dilution activity coefficients

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S1 Experimental techniques in the DECHEMA data collection

Percentage of datapoints in the complete DECHEMA data collection obtained by the experimental techiques: 1) Gas-liquid chromatography with gas phase correction (GLCR), 2) Gas-liquid chromatography with no gas phase correction (GLCI), 3) Gas-liquid chromatography with no specification of gas phase correction (GLCN), 4) Derived from solubility data (SOLU), 5) Dilutor technique (DILU), 6) Static method (STAT), 7) Ebulliometry (EBUL) and 8) other techniques (e.g., liquid-liquid chromatography, derived from Henry coefficients, non-steady-state gas-liquid chromatography, isopiestic technique, dew point technique, relative gas-liquid chromatography and Rayleigh distillation method) (OTHR).

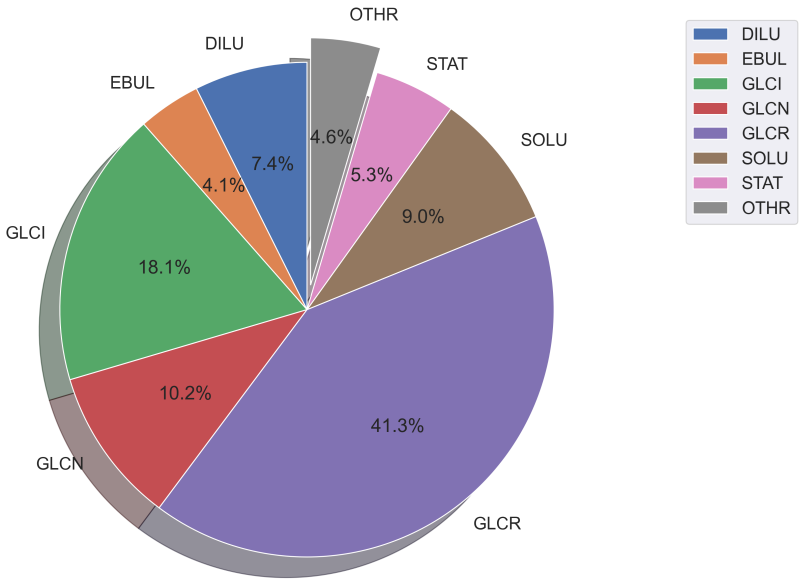

Figure S1: Percentage of datapoints on the complete DECHEMA data collection obtained by different experimental techniques.

S2 Temperature distribution on the DECHEMA dataset

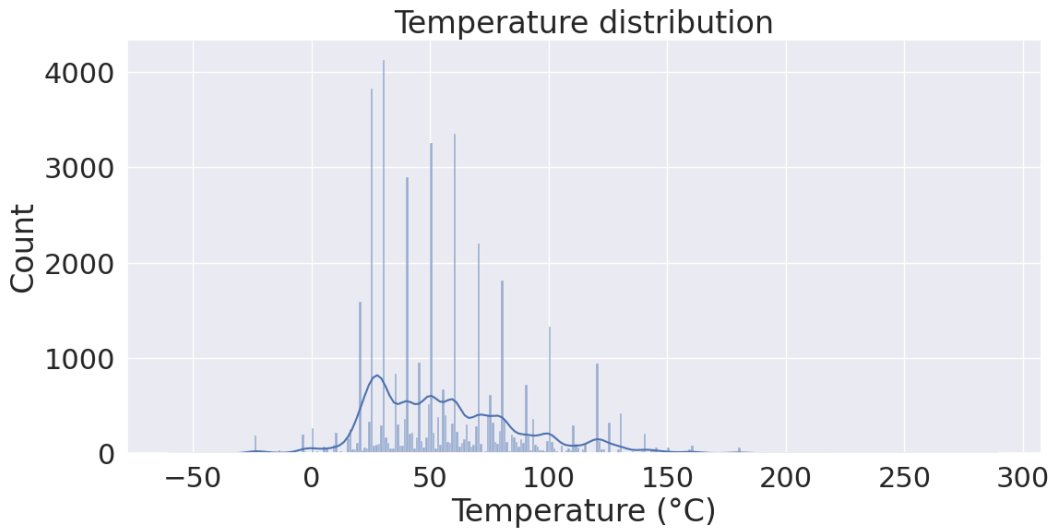

Figure S2: Distribution of temperature values covered in the DECHEMA dataset.

S3 Infinite dilution activity coefficient distribution on the DECHEMA dataset

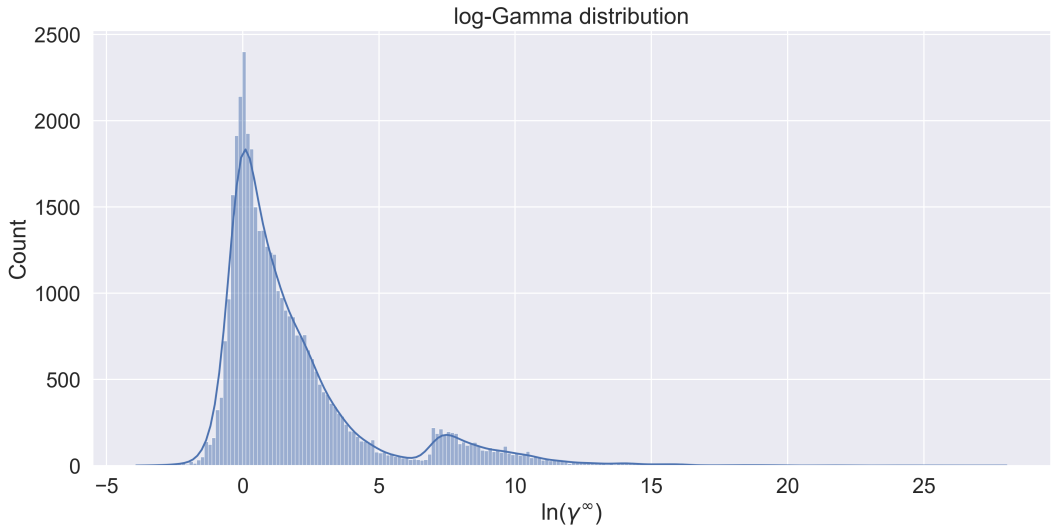

Figure S3: Distribution of $\ln \gamma_{ij}^{\infty}$ values covered in the DECHEMA dataset.

S4 Chemical classes contained in the DECHEMA dataset

These chemical classes were obtained by the Classyfire tool [1] which, to the best of our knowledge, provides the largest and most consistent taxonomy across the chemical space.

Table S1: Chemical classes contained in the DECHEMA dataset obtained from the Classyfire tool [1] along the number of chemical species contained in each class.

Class	No.	Class	No.
Benzene and substituted derivatives	271	Phenanthrenes and derivatives	4
Organooxygen compounds	193	Lactams	4
Fatty Acyls	136	Epoxides	4
Organonitrogen compounds	113	Keto acids and derivatives	3
Carboxylic acids and derivatives	104	Sulfonyls	3
Saturated hydrocarbons	103	Other non-metal organides	3
Unsaturated hydrocarbons	67	Azobenzenes	3
Prenol lipids	39	Dioxanes	3
Organofluorides	32	Homogeneous other non-metal compounds	3
Phenols	30	Pyrroles	3
Organochlorides	28	Oxanes	2
Alkyl halides	27	Dioxolanes	2
Pyridines and derivatives	22	Dihydrofurans	2
Phenol ethers	22	Depsides and depsidones	2
Naphthalenes	20	Thiophenes	2
Organobromides	19	Hydroxy acids and derivatives	2
Allyl-type 1,3-dipolar organic compounds	19	Organic sulfonic acids and derivatives	2
Organic phosphoric acids and derivatives	12	Oxolanes	2
Quinolines and derivatives	12	Organic phosphonic acids and derivatives	2
Thioethers	12	Fluorenes	2
Vinyl halides	12	Organic sulfuric acids and derivatives	2
Thiols	11	Oxathiolanes	2
Heteroaromatic compounds	11	Indoles and derivatives	2
Pyrrolidines	11	Oxathianes	2
Organoiodides	10	Stilbenes	1
Halohydrins	10	Acyl halides	1
Organic oxoanionic compounds	9	Thiophenols	1
Lactones	9	Diarylheptanoids	1

Piperidines	9	Isoquinolines and derivatives	1
Furans	9	Benzofurans	1
Azolidines	9	Aziridines	1
Organo-post-transition metal compounds	9	Organophosphinic acids and derivatives	1
Organometalloid compounds	8	Homogeneous halogens	1
Phenol esters	8	Homogeneous transition metal compounds	1
Oxazinanes	8	Pyrenes	1
Tetrahydrofurans	7	Anthracenes	1
Thiolanes	6	Indanes	1
Azoles	6	Benzothiophenes	1
Sulfoxides	6	Oxacyclic compounds	1
Polycyclic hydrocarbons	6	Tetralins	1
Glycerolipids	6	Indenes and isoindenes	1
Organic carbonic acids and derivatives	5	Organic disulfides	1
Carboximidic acids and derivatives	5	Trialkylphosphites	1
Organic oxides	5	Acyclic allenes	1
Aryl halides	5	Organic metal salts	1
Diazinanes	4		

S5 Hyperparameters for GNNprevious in the isothermal studies

The hyperparameters for GNNprevious were tuned using Optuna [2] by setting the number of trials to 100 and using the corresponding ranges and scales shown in Table S2. For hyperparameter tuning 10-fold cross-validation was used. The final hyperparameters selected for each isothermal study are shown in Table S3. The loss function used was Mean Squared Error (MSE).

Table S2: Ranges used during the hyperparameter search of GNNprevious in the isothermal studies.

Hyperparameter	**Range**	**Search scale**
Message passing layers	2-5	integer
Dropout ratio	0.05-0.5	uniform
Hidden embedding size	16-256	integer
Learning rate	0.0001-1	loguniform
Units in message passing	8-64	integer
Epochs	100-300	integer
Batch size	4-64	integer
Jumping knowledge	{last, sum, mean}	categorical
Global pooling	{sum, mean, max, set2set}	categorical
Hidden layers final MLP	1-2	integer
Units in final MLP	16-128	integer

Table S3: Final selected hyperparameters for GNNprevious in each isothermal study.

Hyperparameter	**Final value for T (C°)**								
	20	25	30	40	50	60	70	80	100
Message passing layers	4	3	4	2	3	3	4	3	5
Dropout ratio	0.13	0.05	0.13	0.05	0.05	0.06	0.05	0.07	0.07
Hidden embedding size	234	41	154	209	72	88	250	64	30
Learning rate	0.002	0.002	0.011	0.003	0.002	0.011	0.001	0.007	0.009
Units in message passing	21	31	18	37	12	42	37	39	10
Epochs	188	239	274	238	168	289	226	144	256
Batch size	39	59	62	44	53	44	42	53	62
Jumping knowledge	last	sum	mean	mean	mean	mean	sum	mean	mean
Global pooling	sum	sum	set2set	sum	sum	sum	sum	sum	mean
Hidden layers final MLP	2	2	1	2	2	2	2	2	2
Units in final MLP	105, 74	83, 30	125	110, 112	104, 126	113, 122	105, 18	97, 56	100, 30

S6 Hyperparameters for SolvGNN in the isothermal studies

The hyperparameters for SolvGNN were tuned using Optuna [2] by setting the number of trials to 100 and using the corresponding ranges and scales shown in Table S4. For hyperparameter tuning 10-fold cross-validation was used. The final hyperparameters selected for each isothermal study are shown in Table S5. The loss function used was Mean Squared Error (MSE).

Table S4: Ranges used during the hyperparameter search of SolvGNN in the isothermal studies.

Hyperparameter	**Range**	**Search scale**
Hidden embedding size	16-256	integer
Learning rate	0.0001-1	loguniform
Epochs	100-300	integer
Batch size	4-64	integer

Table S5: Final selected hyperparameters for SolvGNN in each isothermal study.

Hyperparameter	**Final value for T (C°)**								
	20	25	30	40	50	60	70	80	100
Hidden embedding size	242	226	236	186	197	182	252	162	177
Learning rate	0.0004	0.0004	0.0001	0.0002	0.0006	0.0003	0.0006	0.0002	0.0006
Epochs	156	178	287	151	212	299	256	254	260
Batch size	5	12	4	4	9	7	8	4	4

S7 Hyperparameters for GNNCat, GH-GNN, SolvGNNCat and SolvGNNGH in the temperature dependency studies

The hyperparameters of GNNCat and SolvGNNCat were optimized using Optuna [2] by setting the number of trials to 100, the number of epochs to 50 and using the corresponding ranges and scales shown in Tables S6 and S7. The final hyperparameters selected are also shown in Tables S6 and S7, correspondingly. For hyperparameter tuning 10-fold cross-validation was used with the ranges specified in Table . After the other hyperparameters were selected, the number of epochs were varied over the shown values to select the one that improves the performance on the validation set. The loss function used was Mean Squared Error (MSE). For direct comparison, the hyperparameters of GH-GNN and SolvGNNGH were set to the analogous models GNNCat and SolvGNNCat, respectively. Notice that since GNNCat and SolvGNNCat use only a single multi-layer perceptron (MLP) at the end to predict $\ln \gamma_{ij}^{\infty}$ and to conserved the same number of model parameters between analogous models, the first hidden-layer of the MLP in GNNCat and SolvGNNCat was set to be twice the specified hidden embedding size. The resulting number of model parameters were: 2,483,580 for GNNCat and GH-GNN and 1,798,825 for SolvGNNCat and SolvGNNGH.

Table S6: Ranges used during the hyperparameter search of GNNCat in the temperature dependency studies. The number of epochs was set to 50 for each trial.

Hyperparameter	Range	Search scale	Selected value
Hidden embedding size	16-256	integer	113
Learning rate	0.0001-1	loguniform	0.0002
Epochs	{100, 150, 200, 250, 300}	categorical	250
Batch size	4-64	integer	32

Table S7: Ranges used during the hyperparameter search of SolvGNNCat in the temperature dependency studies. The number of epochs was set to 50 for each trial.

Hyperparameter	Range	Search scale	Selected value
Hidden embedding size	16-256	integer	193
Learning rate	0.0001-1	loguniform	0.00012
Epochs	{100, 150, 200, 250, 300 }	categorical	250
Batch size	4-64	integer	16

S8 Binary systems used for training GH-GNN

Collection of all solvent-solute chemical classes contained in the training set used for developing the GH-GNN model. According to the discussion of the results section in the paper regarding the discrete extrapolation, systems with more than 25 occurrences are expected to produce results with a MAE of approximately 0.3. This systems are marked with a star. "NA" denotes that the class for such compound is "Not-available" according to Classyfire [1].

Table S8: Binary solvent-solute classes contained in the training set used for developing GH-GNN and their occurrences.

No.	Solvent-solute chemical classes	Systems
1	* Benzene and substituted derivatives–Saturated hydrocarbons	876
2	* Organooxygen compounds–Saturated hydrocarbons	596
3	* Benzene and substituted derivatives–Benzene and substituted derivatives	450
4	* Saturated hydrocarbons–Saturated hydrocarbons	395
5	* Organooxygen compounds–Organooxygen compounds	307
6	* Organonitrogen compounds–Saturated hydrocarbons	297
7	* Fatty Acyls–Saturated hydrocarbons	258
8	* Organooxygen compounds–Benzene and substituted derivatives	245
9	* Saturated hydrocarbons–Organooxygen compounds	237
10	* Organooxygen compounds–Unsaturated hydrocarbons	227
11	* Benzene and substituted derivatives–Organooxygen compounds	221
12	* Benzene and substituted derivatives–Unsaturated hydrocarbons	218
13	* Carboxylic acids and derivatives–Saturated hydrocarbons	212
14	* Fatty Acyls–Organooxygen compounds	161
15	* Homogeneous other non-metal compounds–Organooxygen compounds	147
16	* Organonitrogen compounds–Unsaturated hydrocarbons	143
17	* Saturated hydrocarbons–Benzene and substituted derivatives	134
18	* Homogeneous other non-metal compounds–Benzene and substituted derivatives	111
19	* Organonitrogen compounds–Benzene and substituted derivatives	109
20	* Allyl-type 1,3-dipolar organic compounds–Saturated hydrocarbons	108
21	* Fatty Acyls–Benzene and substituted derivatives	108
22	* Carboxylic acids and derivatives–Benzene and substituted derivatives	102
23	* Saturated hydrocarbons–Unsaturated hydrocarbons	95
24	* Naphthalenes–Saturated hydrocarbons	93
25	* Organooxygen compounds–Alkyl halides	93

26	* Benzene and substituted derivatives–Alkyl halides	90
27	* Quinolines and derivatives–Saturated hydrocarbons	89
28	* Carboxylic acids and derivatives–Unsaturated hydrocarbons	86
29	* Fatty Acyls–Carboxylic acids and derivatives	83
30	* Organooxygen compounds–Carboxylic acids and derivatives	81
31	* Organo-post-transition metal compounds–Saturated hydrocarbons	81
32	* Carboxylic acids and derivatives–Organooxygen compounds	78
33	* Homogeneous other non-metal compounds–Fatty Acyls	77
34	* Organooxygen compounds–Organochlorides	76
35	* Pyrrolidines–Saturated hydrocarbons	75
36	* Fatty Acyls–Unsaturated hydrocarbons	74
37	* Pyrrolidines–Unsaturated hydrocarbons	70
38	* Organonitrogen compounds–Organooxygen compounds	70
39	* Homogeneous other non-metal compounds–Carboxylic acids and derivatives	68
40	* Pyridines and derivatives–Saturated hydrocarbons	68
41	* Phenol ethers–Saturated hydrocarbons	68
42	* Saturated hydrocarbons–Carboxylic acids and derivatives	66
43	* Oxazinanes–Saturated hydrocarbons	64
44	* Saturated hydrocarbons–Organochlorides	62
45	* Benzene and substituted derivatives–Organochlorides	62
46	* Carboximidic acids and derivatives–Organooxygen compounds	61
47	* Thiolanes–Saturated hydrocarbons	59
48	* Organic phosphoric acids and derivatives–Saturated hydrocarbons	58
49	* Homogeneous other non-metal compounds–Saturated hydrocarbons	57
50	* Benzene and substituted derivatives–Carboxylic acids and derivatives	56
51	* Phenols–Saturated hydrocarbons	55
52	* Oxazinanes–Unsaturated hydrocarbons	55
53	* Fatty Acyls–Alkyl halides	54
54	* Fatty Acyls–Organochlorides	54
55	* Pyrrolidines–Organooxygen compounds	53
56	* Organic phosphoric acids and derivatives–Organooxygen compounds	53
57	* Saturated hydrocarbons–Organonitrogen compounds	52
58	* Halohydrins–Saturated hydrocarbons	50
59	* Furans–Saturated hydrocarbons	49
60	* Homogeneous other non-metal compounds–Organonitrogen compounds	49
61	* Quinolines and derivatives–Benzene and substituted derivatives	48

62	* Sulfoxides–Saturated hydrocarbons	46
63	* Saturated hydrocarbons–Alkyl halides	45
64	* Prenol lipids–Saturated hydrocarbons	44
65	* Unsaturated hydrocarbons–Benzene and substituted derivatives	44
66	* Prenol lipids–Organooxygen compounds	43
67	* Piperidines–Saturated hydrocarbons	42
68	* Saturated hydrocarbons–Homogeneous other non-metal compounds	42
69	* Organooxygen compounds–Organonitrogen compounds	40
70	* Benzene and substituted derivatives–Organonitrogen compounds	39
71	* Alkyl halides–Saturated hydrocarbons	39
72	* Carboximidic acids and derivatives–Saturated hydrocarbons	39
73	* Azolidines–Unsaturated hydrocarbons	38
74	* Unsaturated hydrocarbons–Saturated hydrocarbons	37
75	* Lactams–Saturated hydrocarbons	35
76	* Azolidines–Saturated hydrocarbons	35
77	* Piperidines–Unsaturated hydrocarbons	32
78	* Tetrahydrofurans–Saturated hydrocarbons	32
79	* Sulfoxides–Unsaturated hydrocarbons	31
80	* Unsaturated hydrocarbons–Organooxygen compounds	31
81	* Allyl-type 1,3-dipolar organic compounds–Benzene and substituted derivatives	31
82	* Organic phosphoric acids and derivatives–Benzene and substituted derivatives	31
83	* Organonitrogen compounds–Alkyl halides	31
84	* Azoles–Saturated hydrocarbons	31
85	* Fatty Acyls–Organonitrogen compounds	31
86	* Organonitrogen compounds–Organochlorides	30
87	* Phenanthrenes and derivatives–Benzene and substituted derivatives	29
88	* Naphthalenes–Benzene and substituted derivatives	29
89	* Carboximidic acids and derivatives–Unsaturated hydrocarbons	29
90	* Organochlorides–Saturated hydrocarbons	28
91	* Organooxygen compounds–Homogeneous other non-metal compounds	28
92	* Organofluorides–Saturated hydrocarbons	28
93	* Phenol ethers–Benzene and substituted derivatives	27
94	* Organochlorides–Organooxygen compounds	27
95	* Thioethers–Saturated hydrocarbons	26
96	* Pyridines and derivatives–Benzene and substituted derivatives	26
97	* Saturated hydrocarbons–Pyridines and derivatives	26

98	* Organooxygen compounds–Organofluorides	26
99	* Organochlorides–Benzene and substituted derivatives	26
100	* Homogeneous other non-metal compounds–Phenols	26
101	* Prenol lipids–Benzene and substituted derivatives	26
102	* Diarylheptanoids–Benzene and substituted derivatives	25
103	* Thiolanes–Benzene and substituted derivatives	25
104	* Thiolanes–Unsaturated hydrocarbons	25
105	* Furans–Unsaturated hydrocarbons	25
106	Saturated hydrocarbons–Organobromides	24
107	Heteroaromatic compounds–Saturated hydrocarbons	24
108	Carboxylic acids and derivatives–Alkyl halides	24
109	Thiolanes–Organooxygen compounds	23
110	Homogeneous other non-metal compounds–Unsaturated hydrocarbons	23
111	Glycerolipids–Organooxygen compounds	23
112	Alkyl halides–Organooxygen compounds	23
113	Pyrrolidines–Benzene and substituted derivatives	22
114	Organic carbonic acids and derivatives–Organooxygen compounds	22
115	Saturated hydrocarbons–Fatty Acyls	22
116	Saturated hydrocarbons–Allyl-type 1,3-dipolar organic compounds	22
117	Organic phosphoric acids and derivatives–Carboxylic acids and derivatives	21
118	Allyl-type 1,3-dipolar organic compounds–Unsaturated hydrocarbons	21
119	Organooxygen compounds–Dioxanes	21
120	Homogeneous other non-metal compounds–Organochlorides	21
121	Organofluorides–Organooxygen compounds	21
122	Organonitrogen compounds–Thioethers	20
123	Benzene and substituted derivatives–Allyl-type 1,3-dipolar organic compounds	20
124	Prenol lipids–Unsaturated hydrocarbons	20
125	Carboxylic acids and derivatives–Carboxylic acids and derivatives	20
126	Diazinanes–Saturated hydrocarbons	20
127	Organooxygen compounds–Allyl-type 1,3-dipolar organic compounds	20
128	Lactones–Saturated hydrocarbons	20
129	Glycerolipids–Prenol lipids	19
130	Organonitrogen compounds–Carboxylic acids and derivatives	19
131	Carboximidic acids and derivatives–Benzene and substituted derivatives	18
132	Organic phosphoric acids and derivatives–Unsaturated hydrocarbons	18
133	Lactams–Unsaturated hydrocarbons	18

134	NA–Saturated hydrocarbons	18
135	Organic carbonic acids and derivatives–Benzene and substituted derivatives	17
136	Organonitrogen compounds–Organonitrogen compounds	17
137	Depsides and depsidones–Saturated hydrocarbons	17
138	Organic metal salts–Saturated hydrocarbons	17
139	Phenols–Benzene and substituted derivatives	17
140	Diazinanes–Unsaturated hydrocarbons	17
141	Organobromides–Saturated hydrocarbons	17
142	Oxazinanes–Benzene and substituted derivatives	17
143	Organo-post-transition metal compounds–Benzene and substituted derivatives	17
144	Oxazinanes–Organooxygen compounds	16
145	Dioxanes–Saturated hydrocarbons	16
146	Organooxygen compounds–Naphthalenes	16
147	Isoquinolines and derivatives–Saturated hydrocarbons	16
148	Organochlorides–Organochlorides	16
149	Unsaturated hydrocarbons–Unsaturated hydrocarbons	16
150	Organochlorides–Alkyl halides	16
151	Carboximidic acids and derivatives–Carboxylic acids and derivatives	16
152	Lactones–Organooxygen compounds	16
153	Saturated hydrocarbons–NA	15
154	Benzene and substituted derivatives–Fatty Acyls	15
155	Azoles–Unsaturated hydrocarbons	15
156	Saturated hydrocarbons–Organofluorides	15
157	Organic phosphoric acids and derivatives–Alkyl halides	15
158	Unsaturated hydrocarbons–Carboxylic acids and derivatives	15
159	Phenol ethers–Unsaturated hydrocarbons	14
160	Piperidines–Organooxygen compounds	14
161	Organic carbonic acids and derivatives–Saturated hydrocarbons	14
162	Benzene and substituted derivatives–Heteroaromatic compounds	14
163	Lactams–Benzene and substituted derivatives	14
164	Naphthalenes–Unsaturated hydrocarbons	14
165	Diarylheptanoids–Saturated hydrocarbons	14
166	Alkyl halides–Benzene and substituted derivatives	14
167	Organooxygen compounds–Fatty Acyls	14
168	Homogeneous other non-metal compounds–Alkyl halides	14
169	Azolidines–Organooxygen compounds	14

170	Homogeneous other non-metal compounds–Prenol lipids	13
171	NA–Unsaturated hydrocarbons	13
172	Prenol lipids–Organochlorides	13
173	Prenol lipids–Carboxylic acids and derivatives	13
174	Tetrahydrofurans–Unsaturated hydrocarbons	13
175	Naphthalenes–Organooxygen compounds	13
176	Saturated hydrocarbons–Organoiodides	13
177	Sulfoxides–Organooxygen compounds	13
178	Prenol lipids–Pyridines and derivatives	13
179	NA–Organooxygen compounds	13
180	Organobromides–Benzene and substituted derivatives	13
181	Sulfonyls–Saturated hydrocarbons	13
182	Prenol lipids–Alkyl halides	13
183	Benzene and substituted derivatives–Dioxanes	12
184	Organometalloid compounds–Saturated hydrocarbons	12
185	Sulfoxides–Benzene and substituted derivatives	12
186	Organooxygen compounds–Organo-post-transition metal compounds	12
187	Halohydrins–Unsaturated hydrocarbons	12
188	Prenol lipids–Heteroaromatic compounds	12
189	Quinolines and derivatives–Unsaturated hydrocarbons	12
190	Benzene and substituted derivatives–Vinyl halides	12
191	Depsides and depsidones–Benzene and substituted derivatives	12
192	Alkyl halides–Organochlorides	12
193	Organooxygen compounds–Vinyl halides	12
194	Sulfonyls–Unsaturated hydrocarbons	11
195	Azobenzenes–Benzene and substituted derivatives	11
196	Organooxygen compounds–Heteroaromatic compounds	11
197	Organonitrogen compounds–NA	11
198	Lactones–Unsaturated hydrocarbons	11
199	Fluorenes–Benzene and substituted derivatives	11
200	Saturated hydrocarbons–Phenols	11
201	Furans–Benzene and substituted derivatives	11
202	Phenol ethers–Organochlorides	11
203	Lactones–Benzene and substituted derivatives	11
204	Organonitrogen compounds–Heteroaromatic compounds	11
205	Organooxygen compounds–Organoiodides	11

206	Carboxylic acids and derivatives–Organochlorides	10
207	Organooxygen compounds–Tetrahydrofurans	10
208	Carboximidic acids and derivatives–Alkyl halides	10
209	Organoiodides–Benzene and substituted derivatives	10
210	Phenols–Unsaturated hydrocarbons	10
211	Homogeneous other non-metal compounds–Organobromides	10
212	Organochlorides–Unsaturated hydrocarbons	10
213	Alkyl halides–Organonitrogen compounds	10
214	Other non-metal organides–Saturated hydrocarbons	10
215	Fatty Acyls–Vinyl halides	10
216	Alkyl halides–Alkyl halides	10
217	Thiols–Saturated hydrocarbons	10
218	Phenol esters–Saturated hydrocarbons	10
219	Organooxygen compounds–Phenanthrenes and derivatives	10
220	Pyrrolidines–Alkyl halides	10
221	Phenanthrenes and derivatives–Saturated hydrocarbons	9
222	Heteroaromatic compounds–Unsaturated hydrocarbons	9
223	Benzene and substituted derivatives–Thioethers	9
224	Saturated hydrocarbons–Tetrahydrofurans	9
225	Homogeneous other non-metal compounds–Phenol ethers	9
226	Glycerolipids–Benzene and substituted derivatives	9
227	Organic sulfonic acids and derivatives–Saturated hydrocarbons	9
228	Halohydrins–Benzene and substituted derivatives	9
229	Saturated hydrocarbons–Organo-post-transition metal compounds	9
230	Organochlorides–Organonitrogen compounds	9
231	Homogeneous other non-metal compounds–Vinyl halides	9
232	Keto acids and derivatives–Saturated hydrocarbons	9
233	Oxathiolanes–Saturated hydrocarbons	9
234	Alkyl halides–Vinyl halides	9
235	Organofluorides–Benzene and substituted derivatives	8
236	Benzene and substituted derivatives–Other non-metal organides	8
237	Benzene and substituted derivatives–Organobromides	8
238	Glycerolipids–Saturated hydrocarbons	8
239	Polycyclic hydrocarbons–Saturated hydrocarbons	8
240	Tetrahydrofurans–Benzene and substituted derivatives	8
241	Fatty Acyls–Allyl-type 1,3-dipolar organic compounds	8

242	Carboxylic acids and derivatives–Organonitrogen compounds	8
243	Piperidines–Benzene and substituted derivatives	8
244	Organooxygen compounds–Pyridines and derivatives	8
245	Azolidines–Benzene and substituted derivatives	8
246	Tetrahydrofurans–Organooxygen compounds	8
247	Homogeneous other non-metal compounds–NA	8
248	Oxolanes–Saturated hydrocarbons	8
249	Allyl-type 1,3-dipolar organic compounds–Alkyl halides	8
250	Benzene and substituted derivatives–Organoiodides	8
251	Thioethers–Benzene and substituted derivatives	8
252	NA–Benzene and substituted derivatives	8
253	Carboxylic acids and derivatives–Tetrahydrofurans	8
254	Phenol esters–Benzene and substituted derivatives	7
255	Prenol lipids–Organic oxoanionic compounds	7
256	Diarylheptanoids–Unsaturated hydrocarbons	7
257	Glycerolipids–Organochlorides	7
258	Thiophenols–Saturated hydrocarbons	7
259	Glycerolipids–Carboxylic acids and derivatives	7
260	Glycerolipids–Alkyl halides	7
261	Benzene and substituted derivatives–NA	7
262	Benzene and substituted derivatives–Prenol lipids	7
263	Fatty Acyls–Organofluorides	7
264	Benzene and substituted derivatives–Tetrahydrofurans	7
265	Carboxylic acids and derivatives–Heteroaromatic compounds	7
266	Acyl halides–Saturated hydrocarbons	7
267	Azobenzenes–Saturated hydrocarbons	7
268	Azoles–Benzene and substituted derivatives	7
269	Carboxylic acids and derivatives–NA	7
270	Carboximidic acids and derivatives–Organonitrogen compounds	7
271	Allyl-type 1,3-dipolar organic compounds–Organooxygen compounds	7
272	Diarylheptanoids–Organochlorides	7
273	Saturated hydrocarbons–Pyrrolidines	7
274	Benzene and substituted derivatives–Homogeneous other non-metal compounds	7
275	Phenol ethers–Alkyl halides	7
276	Oxazinanes–NA	7
277	Diarylheptanoids–Alkyl halides	7

278	Dioxolanes–Saturated hydrocarbons	7
279	Thiolanes–Carboxylic acids and derivatives	6
280	NA–Alkyl halides	6
281	Organic sulfuric acids and derivatives–Saturated hydrocarbons	6
282	Organochlorides–Vinyl halides	6
283	Diarylheptanoids–Organooxygen compounds	6
284	Thiolanes–Thioethers	6
285	Phenol ethers–Organooxygen compounds	6
286	Pyrrolidines–NA	6
287	Organochlorides–Homogeneous other non-metal compounds	6
288	Organooxygen compounds–Anthracenes	6
289	Organooxygen compounds–Tetralins	6
290	Prenol lipids–Organonitrogen compounds	6
291	Prenol lipids–Tetrahydrofurans	6
292	Organooxygen compounds–Organobromides	6
293	Prenol lipids–Phenol esters	6
294	Saturated hydrocarbons–Thiols	6
295	NA–Carboxylic acids and derivatives	6
296	Quinolines and derivatives–Organooxygen compounds	6
297	Organic phosphoric acids and derivatives–Homogeneous other non-metal compounds	6
298	Thioethers–Unsaturated hydrocarbons	6
299	Hydroxy acids and derivatives–Organooxygen compounds	6
300	Unsaturated hydrocarbons–Organochlorides	6
301	Organic sulfonic acids and derivatives–Unsaturated hydrocarbons	6
302	Hydroxy acids and derivatives–Benzene and substituted derivatives	6
303	Unsaturated hydrocarbons–Allyl-type 1,3-dipolar organic compounds	6
304	Fatty Acyls–Tetrahydrofurans	6
305	Hydroxy acids and derivatives–Saturated hydrocarbons	6
306	Benzene and substituted derivatives–Phenol esters	6
307	Acyl halides–Organooxygen compounds	6
308	Organo-post-transition metal compounds–Unsaturated hydrocarbons	6
309	Carboximidic acids and derivatives–Organochlorides	6
310	Naphthalenes–Alkyl halides	6
311	Organooxygen compounds–Thioethers	6
312	Organochlorides–Carboxylic acids and derivatives	6
313	Saturated hydrocarbons–Prenol lipids	5

314	Alkyl halides–Carboxylic acids and derivatives	5
315	Homogeneous other non-metal compounds–Pyridines and derivatives	5
316	Stilbenes–Benzene and substituted derivatives	5
317	Unsaturated hydrocarbons–Alkyl halides	5
318	Fatty Acyls–Fatty Acyls	5
319	Carboxylic acids and derivatives–Dioxanes	5
320	Homogeneous other non-metal compounds–Naphthalenes	5
321	Organonitrogen compounds–Thiolanes	5
322	Unsaturated hydrocarbons–Organonitrogen compounds	5
323	Glycerolipids–Organofluorides	5
324	Organochlorides–Allyl-type 1,3-dipolar organic compounds	5
325	Benzene and substituted derivatives–Carboximidic acids and derivatives	5
326	Saturated hydrocarbons–Lactams	5
327	Benzene and substituted derivatives–Organic oxoanionic compounds	5
328	Prenol lipids–Allyl-type 1,3-dipolar organic compounds	5
329	Oxolanes–Unsaturated hydrocarbons	5
330	Homogeneous other non-metal compounds–Allyl-type 1,3-dipolar organic compounds	5
331	Organic phosphoric acids and derivatives–Organochlorides	5
332	Pyrrolidines–Carboxylic acids and derivatives	5
333	Prenol lipids–Fatty Acyls	5
334	Fluorenes–Saturated hydrocarbons	5
335	Benzofurans–Saturated hydrocarbons	5
336	Saturated hydrocarbons–Vinyl halides	5
337	Azolidines–NA	5
338	Oxazinanes–Carboxylic acids and derivatives	5
339	Organoiodides–Saturated hydrocarbons	5
340	Prenol lipids–Phenols	5
341	Organic phosphoric acids and derivatives–Phenol esters	4
342	Organic phosphoric acids and derivatives–Dioxanes	4
343	Benzene and substituted derivatives–Aryl halides	4
344	Acyl halides–Carboxylic acids and derivatives	4
345	Organofluorides–Unsaturated hydrocarbons	4
346	Phenols–Organochlorides	4
347	Alkyl halides–Organoiodides	4
348	Phenols–Naphthalenes	4
349	Alkyl halides–Organo-post-transition metal compounds	4

350	Saturated hydrocarbons–Dioxanes	4
351	Acyl halides–Unsaturated hydrocarbons	4
352	Saturated hydrocarbons–Other non-metal organides	4
353	Sulfonyls–Benzene and substituted derivatives	4
354	Allyl-type 1,3-dipolar organic compounds–Organochlorides	4
355	Vinyl halides–Benzene and substituted derivatives	4
356	Prenol lipids–Aryl halides	4
357	Saturated hydrocarbons–Polycyclic hydrocarbons	4
358	Vinyl halides–Organochlorides	4
359	Thiolanes–Thiols	4
360	Organooxygen compounds–Polycyclic hydrocarbons	4
361	Tetrahydrofurans–Alkyl halides	4
362	Saturated hydrocarbons–Oxazinanes	4
363	Saturated hydrocarbons–Thioethers	4
364	Saturated hydrocarbons–Heteroaromatic compounds	4
365	Pyridines and derivatives–Unsaturated hydrocarbons	4
366	Alkyl halides–Allyl-type 1,3-dipolar organic compounds	4
367	Pyridines and derivatives–Organooxygen compounds	4
368	Polycyclic hydrocarbons–Unsaturated hydrocarbons	4
369	Alkyl halides–Homogeneous other non-metal compounds	4
370	Dioxanes–Unsaturated hydrocarbons	4
371	Dioxolanes–Unsaturated hydrocarbons	4
372	Naphthalenes–Carboxylic acids and derivatives	4
373	Naphthalenes–Organonitrogen compounds	4
374	Organonitrogen compounds–Thiols	4
375	Organonitrogen compounds–Phenol esters	4
376	Thiolanes–Heteroaromatic compounds	4
377	Benzene and substituted derivatives–Organo-post-transition metal compounds	4
378	Organonitrogen compounds–Other non-metal organides	4
379	Organonitrogen compounds–Dioxanes	4
380	Diarylheptanoids–Carboxylic acids and derivatives	4
381	Carboxylic acids and derivatives–Homogeneous other non-metal compounds	4
382	Thiols–Organooxygen compounds	4
383	Organic carbonic acids and derivatives–Organochlorides	4
384	Organic carbonic acids and derivatives–Organonitrogen compounds	4
385	Organic oxides–Unsaturated hydrocarbons	4

386	Benzene and substituted derivatives–Thiols	4
387	Glycerolipids–Fatty Acyls	4
388	Organic carbonic acids and derivatives–Carboxylic acids and derivatives	4
389	Organic oxides–Saturated hydrocarbons	4
390	Unsaturated hydrocarbons–Prenol lipids	4
391	Organooxygen compounds–Thiols	4
392	Carboxylic acids and derivatives–Allyl-type 1,3-dipolar organic compounds	4
393	Dioxanes–Benzene and substituted derivatives	4
394	Sulfoxides–Carboxylic acids and derivatives	4
395	Carboxylic acids and derivatives–Other non-metal organides	4
396	Organooxygen compounds–Other non-metal organides	4
397	Sulfoxides–Acyclic allenes	4
398	Fatty Acyls–Homogeneous other non-metal compounds	4
399	Fatty Acyls–Phenol ethers	4
400	Organonitrogen compounds–Allyl-type 1,3-dipolar organic compounds	4
401	Organonitrogen compounds–Phenols	4
402	Organooxygen compounds–Prenol lipids	4
403	Tetralins–Unsaturated hydrocarbons	4
404	Organochlorides–Organo-post-transition metal compounds	4
405	Glycerolipids–Heteroaromatic compounds	4
406	Organofluorides–Organofluorides	4
407	Organic carbonic acids and derivatives–Alkyl halides	4
408	Organooxygen compounds–Organometalloid compounds	4
409	Organooxygen compounds–Phenols	4
410	Alkyl halides–Tetrahydrofurans	3
411	Organonitrogen compounds–Organobromides	3
412	Carboxylic acids and derivatives–Organofluorides	3
413	Benzene and substituted derivatives–Phenol ethers	3
414	Quinolines and derivatives–Alkyl halides	3
415	Organofluorides–Carboxylic acids and derivatives	3
416	Prenol lipids–Phenol ethers	3
417	Carboximidic acids and derivatives–Tetrahydrofurans	3
418	Alkyl halides–Organofluorides	3
419	Homogeneous other non-metal compounds–Heteroaromatic compounds	3
420	Organofluorides–Alkyl halides	3
421	Organo-post-transition metal compounds–Alkyl halides	3

422	Other non-metal organides–Organooxygen compounds	3
423	Phenols–Organooxygen compounds	3
424	Homogeneous other non-metal compounds–Quinolines and derivatives	3
425	Pyrrolidines–Tetrahydrofurans	3
426	Piperidines–Carboxylic acids and derivatives	3
427	Prenol lipids–Vinyl halides	3
428	Vinyl halides–Unsaturated hydrocarbons	3
429	Vinyl halides–Homogeneous other non-metal compounds	3
430	Vinyl halides–Alkyl halides	3
431	Vinyl halides–Vinyl halides	3
432	Azolidines–Carboxylic acids and derivatives	3
433	Heteroaromatic compounds–Benzene and substituted derivatives	3
434	Vinyl halides–Saturated hydrocarbons	3
435	Homogeneous other non-metal compounds–Thiols	3
436	Hydroxy acids and derivatives–Unsaturated hydrocarbons	3
437	Organoiodides–Alkyl halides	3
438	Organic metal salts–Benzene and substituted derivatives	3
439	Saturated hydrocarbons–Halohydrins	3
440	Hydroxy acids and derivatives–Organochlorides	3
441	Allyl-type 1,3-dipolar organic compounds–Organoiodides	3
442	Acyl halides–Organochlorides	3
443	Phenanthrenes and derivatives–Organooxygen compounds	3
444	Phenols–Alkyl halides	3
445	Oxathiolanes–Unsaturated hydrocarbons	3
446	Acyl halides–Organonitrogen compounds	3
447	Hydroxy acids and derivatives–Organonitrogen compounds	3
448	Glycerolipids–Tetrahydrofurans	3
449	Sulfoxides–Alkyl halides	3
450	Unsaturated hydrocarbons–Homogeneous other non-metal compounds	3
451	Saturated hydrocarbons–Carboximidic acids and derivatives	3
452	Benzofurans–Benzene and substituted derivatives	3
453	Thiolanes–NA	3
454	Saturated hydrocarbons–Thiolanes	3
455	NA–Organochlorides	3
456	Glycerolipids–Vinyl halides	3
457	Glycerolipids–Allyl-type 1,3-dipolar organic compounds	3

458	Organic carbonic acids and derivatives–Unsaturated hydrocarbons	3
459	Saturated hydrocarbons–Sulfoxides	3
460	Benzene and substituted derivatives–Pyridines and derivatives	3
461	Thiolanes–Polycyclic hydrocarbons	3
462	Organooxygen compounds–NA	3
463	Organic phosphoric acids and derivatives–Organonitrogen compounds	3
464	Fatty Acyls–Organobromides	3
465	Diarylheptanoids–Vinyl halides	3
466	Depsides and depsidones–Organooxygen compounds	3
467	Hydroxy acids and derivatives–Carboxylic acids and derivatives	3
468	Thiolanes–Alkyl halides	3
469	Diazinanes–Benzene and substituted derivatives	3
470	Indenes and isoindenes–Saturated hydrocarbons	3
471	Homogeneous other non-metal compounds–Organoiodides	3
472	Saturated hydrocarbons–Naphthalenes	3
473	Benzene and substituted derivatives–Organometalloid compounds	3
474	Dioxolanes–Benzene and substituted derivatives	2
475	Heteroaromatic compounds–NA	2
476	Naphthalenes–Pyridines and derivatives	2
477	Naphthalenes–Allyl-type 1,3-dipolar organic compounds	2
478	Dioxanes–Organooxygen compounds	2
479	Naphthalenes–Organochlorides	2
480	Oxathiolanes–Benzene and substituted derivatives	2
481	Piperidines–Alkyl halides	2
482	Fatty Acyls–Heteroaromatic compounds	2
483	Homogeneous other non-metal compounds–Piperidines	2
484	Homogeneous other non-metal compounds–Organic phosphonic acids and derivatives	2
485	Homogeneous other non-metal compounds–Lactones	2
486	Organonitrogen compounds–Organometalloid compounds	2
487	Acyl halides–Benzene and substituted derivatives	2
488	NA–Pyrrolidines	2
489	NA–Sulfoxides	2
490	Lactams–Prenol lipids	2
491	Thiols–Carboxylic acids and derivatives	2
492	Homogeneous other non-metal compounds–Organometalloid compounds	2
493	Homogeneous other non-metal compounds–Organic oxides	2

494	Acyl halides–Alkyl halides	2
495	Isoquinolines and derivatives–Unsaturated hydrocarbons	2
496	Quinolines and derivatives–Organochlorides	2
497	Hydroxy acids and derivatives–Alkyl halides	2
498	Pyridines and derivatives–Homogeneous other non-metal compounds	2
499	Lactones–Alkyl halides	2
500	Allyl-type 1,3-dipolar organic compounds–Other non-metal organides	2
501	Thiols–Unsaturated hydrocarbons	2
502	Allyl-type 1,3-dipolar organic compounds–Organobromides	2
503	Phenanthrenes and derivatives–Unsaturated hydrocarbons	2
504	Halohydrins–NA	2
505	Pyridines and derivatives–Allyl-type 1,3-dipolar organic compounds	2
506	Pyrroles–Benzene and substituted derivatives	2
507	Alkyl halides–Dioxanes	2
508	Unsaturated hydrocarbons–Pyrrolidines	2
509	NA–Thiolanes	2
510	Saturated hydrocarbons–Phenol ethers	2
511	Pyridines and derivatives–Dioxanes	2
512	Lactones–Carboxylic acids and derivatives	2
513	Tetrahydrofurans–Carboxylic acids and derivatives	2
514	Sulfoxides–NA	2
515	Tetralins–Saturated hydrocarbons	2
516	Homogeneous other non-metal compounds–Oxanes	2
517	Organic phosphoric acids and derivatives–Other non-metal organides	2
518	Organochlorides–Organobromides	2
519	Benzene and substituted derivatives–Phenols	2
520	Phenol ethers–Vinyl halides	2
521	Organic sulfonic acids and derivatives–Benzene and substituted derivatives	2
522	Organic sulfuric acids and derivatives–Benzene and substituted derivatives	2
523	Organic phosphoric acids and derivatives–Phenols	2
524	Benzofurans–Organooxygen compounds	2
525	Thiophenols–Benzene and substituted derivatives	2
526	Organic phosphoric acids and derivatives–Organometalloid compounds	2
527	NA–Organonitrogen compounds	2
528	Phenol ethers–Prenol lipids	2
529	Phenol esters–Unsaturated hydrocarbons	2

530	Thiolanes–Prenol lipids	2
531	Thiolanes–Organochlorides	2
532	Benzene and substituted derivatives–Thiolanes	2
533	Organometalloid compounds–Homogeneous other non-metal compounds	2
534	Benzene and substituted derivatives–Organofluorides	2
535	Diarylheptanoids–Organonitrogen compounds	2
536	Saturated hydrocarbons–Dioxolanes	2
537	Organochlorides–Organoiodides	2
538	Keto acids and derivatives–Unsaturated hydrocarbons	2
539	Piperidines–NA	2
540	Glycerolipids–Phenol ethers	2
541	Other non-metal organides–Benzene and substituted derivatives	2
542	Glycerolipids–Unsaturated hydrocarbons	2
543	Organobromides–Homogeneous other non-metal compounds	2
544	Organonitrogen compounds–Tetrahydrofurans	2
545	Fluorenes–Organonitrogen compounds	2
546	Prenol lipids–Organobromides	2
547	Pyrrolidines–Prenol lipids	2
548	Thiols–Benzene and substituted derivatives	2
549	Organic oxides–Benzene and substituted derivatives	2
550	Oxazinanes–Acyclic allenes	2
551	Organonitrogen compounds–Pyridines and derivatives	2
552	Carboxylic acids and derivatives–Vinyl halides	2
553	Carboxylic acids and derivatives–Pyridines and derivatives	2
554	Phenols–Phenanthrenes and derivatives	2
555	Homogeneous other non-metal compounds–Organo-post-transition metal compounds	2
556	Prenol lipids–Organometalloid compounds	2
557	Homogeneous other non-metal compounds–Tetrahydrofurans	2
558	Organochlorides–Tetrahydrofurans	2
559	Homogeneous other non-metal compounds–Indoles and derivatives	2
560	Carboxylic acids and derivatives–Organoiodides	2
561	Carboxylic acids and derivatives–Organobromides	2
562	Fluorenes–Organooxygen compounds	2
563	Carboximidic acids and derivatives–Fatty Acyls	2
564	Organonitrogen compounds–Homogeneous other non-metal compounds	2
565	Pyrrolidines–Homogeneous other non-metal compounds	2

566	Organonitrogen compounds–Organoiodides	2
567	Dioxanes–Alkyl halides	2
568	Homogeneous other non-metal compounds–Organic phosphoric acids and derivatives	1
569	Piperidines–Homogeneous other non-metal compounds	1
570	Homogeneous other non-metal compounds–Tetralins	1
571	Hydroxy acids and derivatives–Homogeneous other non-metal compounds	1
572	Organobromides–Carboxylic acids and derivatives	1
573	Organobromides–Organochlorides	1
574	Homogeneous other non-metal compounds–Organic oxoanionic compounds	1
575	Organobromides–Organonitrogen compounds	1
576	Hydroxy acids and derivatives–Allyl-type 1,3-dipolar organic compounds	1
577	Homogeneous other non-metal compounds–Homogeneous other non-metal compounds	1
578	Homogeneous other non-metal compounds–Indanes	1
579	Homogeneous other non-metal compounds–Homogeneous halogens	1
580	Homogeneous other non-metal compounds–Thioethers	1
581	Homogeneous other non-metal compounds–Homogeneous transition metal compounds	1
582	Homogeneous other non-metal compounds–Sulfoxides	1
583	Pyrroles–Saturated hydrocarbons	1
584	Thiolanes–Indenes and isoindenes	1
585	Homogeneous other non-metal compounds–Epoxides	1
586	Homogeneous other non-metal compounds–Dioxanes	1
587	Organooxygen compounds–Indenes and isoindenes	1
588	Sulfonyls–Acyclic allenes	1
589	Organooxygen compounds–Organic sulfuric acids and derivatives	1
590	Benzene and substituted derivatives–Oxacyclic compounds	1
591	Phenols–Allyl-type 1,3-dipolar organic compounds	1
592	Tetralins–Benzene and substituted derivatives	1
593	Tetralins–NA	1
594	Thiolanes–Other non-metal organides	1
595	Thiolanes–Dioxanes	1
596	Sulfoxides–Homogeneous other non-metal compounds	1
597	Sulfoxides–Heteroaromatic compounds	1
598	Sulfoxides–Organo-post-transition metal compounds	1
599	Sulfoxides–Pyrrolidines	1
600	Sulfoxides–Allyl-type 1,3-dipolar organic compounds	1
601	Sulfoxides–Tetrahydrofurans	1

602	Sulfoxides–Organoiodides	1
603	Sulfoxides–Organochlorides	1
604	Thiolanes–Organonitrogen compounds	1
605	Sulfoxides–Organonitrogen compounds	1
606	Diazinanes–NA	1
607	Sulfoxides–Dioxanes	1
608	Thiolanes–Homogeneous other non-metal compounds	1
609	Thiolanes–Thiolanes	1
610	Thiolanes–Tetralins	1
611	Thiolanes–Pyridines and derivatives	1
612	Thiolanes–Oxanes	1
613	Thiolanes–Vinyl halides	1
614	Thiolanes–Tetrahydrofurans	1
615	Thiolanes–Naphthalenes	1
616	Organooxygen compounds–Thiolanes	1
617	Organo-post-transition metal compounds–Organochlorides	1
618	Homogeneous other non-metal compounds–Organic disulfides	1
619	Homogeneous other non-metal compounds–Halohydrins	1
620	Homogeneous other non-metal compounds–Organophosphinic acids and derivatives	1
621	Homogeneous other non-metal compounds–Dioxolanes	1
622	Pyridines and derivatives–NA	1
623	Pyridines and derivatives–Carboximidic acids and derivatives	1
624	Quinolines and derivatives–NA	1
625	Homogeneous other non-metal compounds–Other non-metal organides	1
626	Quinolines and derivatives–Carboxylic acids and derivatives	1
627	Quinolines and derivatives–Organonitrogen compounds	1
628	Quinolines and derivatives–Organobromides	1
629	Quinolines and derivatives–Organoiodides	1
630	Homogeneous other non-metal compounds–Keto acids and derivatives	1
631	Homogeneous other non-metal compounds–Phenanthrenes and derivatives	1
632	Organometalloid compounds–Unsaturated hydrocarbons	1
633	Organometalloid compounds–Benzene and substituted derivatives	1
634	Homogeneous other non-metal compounds–Pyrenes	1
635	Prenol lipids–Dioxanes	1
636	Prenol lipids–Pyrrolidines	1
637	Homogeneous other non-metal compounds–Benzothiophenes	1

638	Prenol lipids–Other non-metal organides	1
639	Prenol lipids–Organic carbonic acids and derivatives	1
640	Homogeneous other non-metal compounds–Anthracenes	1
641	Homogeneous other non-metal compounds–Phenol esters	1
642	Homogeneous other non-metal compounds–Carboximidic acids and derivatives	1
643	Homogeneous other non-metal compounds–Glycerolipids	1
644	Prenol lipids–Organic phosphoric acids and derivatives	1
645	Prenol lipids–Trialkylphosphites	1
646	Prenol lipids–Sulfoxides	1
647	Prenol lipids–Thiophenes	1
648	Organic metal salts–Unsaturated hydrocarbons	1
649	Homogeneous other non-metal compounds–Pyrrolidines	1
650	NA–Pyridines and derivatives	1
651	Benzene and substituted derivatives–Thiophenes	1
652	Carboximidic acids and derivatives–Pyridines and derivatives	1
653	Organonitrogen compounds–Naphthalenes	1
654	Phenol ethers–Phenol ethers	1
655	Organonitrogen compounds–Organofluorides	1
656	Organonitrogen compounds–Phenol ethers	1
657	Organonitrogen compounds–Carboximidic acids and derivatives	1
658	Organonitrogen compounds–Organo-post-transition metal compounds	1
659	Organonitrogen compounds–Oxacyclic compounds	1
660	Carboxylic acids and derivatives–Organo-post-transition metal compounds	1
661	Carboximidic acids and derivatives–Homogeneous other non-metal compounds	1
662	Carboximidic acids and derivatives–Phenols	1
663	Depsides and depsidones–Organonitrogen compounds	1
664	Carboximidic acids and derivatives–Naphthalenes	1
665	Carboximidic acids and derivatives–Heteroaromatic compounds	1
666	Carboximidic acids and derivatives–Vinyl halides	1
667	Carboximidic acids and derivatives–Dioxanes	1
668	Quinolines and derivatives–Phenol ethers	1
669	Oxazinanes–Heteroaromatic compounds	1
670	Oxazinanes–Tetrahydrofurans	1
671	Oxazinanes–Fatty Acyls	1
672	Oxazinanes–Dioxanes	1
673	Depsides and depsidones–Carboxylic acids and derivatives	1

674	Depsides and depsidones–Organochlorides	1
675	Dihydrofurans–Saturated hydrocarbons	1
676	Phenol ethers–Organoiodides	1
677	Diarylheptanoids–Allyl-type 1,3-dipolar organic compounds	1
678	Diarylheptanoids–Organic carbonic acids and derivatives	1
679	Diarylheptanoids–Other non-metal organides	1
680	Diarylheptanoids–Phenol ethers	1
681	Benzene and substituted derivatives–Lactams	1
682	Benzene and substituted derivatives–Pyrrolidines	1
683	Phenol ethers–Other non-metal organides	1
684	Phenol ethers–Allyl-type 1,3-dipolar organic compounds	1
685	Phenol ethers–Dioxanes	1
686	Phenol ethers–Organobromides	1
687	Depsides and depsidones–Fatty Acyls	1
688	Phenol ethers–Organonitrogen compounds	1
689	Phenol ethers–Carboxylic acids and derivatives	1
690	Benzene and substituted derivatives–Naphthalenes	1
691	Phenol esters–Fatty Acyls	1
692	Phenol esters–Organochlorides	1
693	Phenol esters–Organonitrogen compounds	1
694	Phenol esters–Carboxylic acids and derivatives	1
695	Phenol esters–Organooxygen compounds	1
696	Depsides and depsidones–Unsaturated hydrocarbons	1
697	Oxolanes–Benzene and substituted derivatives	1
698	Dihydrofurans–Benzene and substituted derivatives	1
699	Keto acids and derivatives–Benzene and substituted derivatives	1
700	Oxathianes–Saturated hydrocarbons	1
701	Fatty Acyls–Other non-metal organides	1
702	Fatty Acyls–Dioxanes	1
703	Unsaturated hydrocarbons–Heteroaromatic compounds	1
704	Unsaturated hydrocarbons–Organobromides	1
705	Aziridines–Saturated hydrocarbons	1
706	Aziridines–Benzene and substituted derivatives	1
707	Thiols–Alkyl halides	1
708	Thiols–Organochlorides	1
709	Thiols–Organonitrogen compounds	1

710	Oxathianes–Benzene and substituted derivatives	1
711	Fatty Acyls–Halohydrins	1
712	Oxathianes–Unsaturated hydrocarbons	1
713	Dioxanes–Phenols	1
714	Dioxanes–Allyl-type 1,3-dipolar organic compounds	1
715	Dioxanes–Organoiodides	1
716	Dioxanes–Organonitrogen compounds	1
717	Carboxylic acids and derivatives–Phenol ethers	1
718	Organic carbonic acids and derivatives–Organo-post-transition metal compounds	1
719	Organic carbonic acids and derivatives–Organoiodides	1
720	Organic carbonic acids and derivatives–Homogeneous other non-metal compounds	1
721	Fatty Acyls–Organoiodides	1
722	Fatty Acyls–Epoxides	1
723	Pyrrolidines–Heteroaromatic compounds	1
724	Halohydrins–Dioxanes	1
725	Pyrrolidines–Organo-post-transition metal compounds	1
726	Pyrrolidines–Allyl-type 1,3-dipolar organic compounds	1
727	Pyrrolidines–Other non-metal organides	1
728	Pyrrolidines–Fatty Acyls	1
729	Pyrrolidines–Polycyclic hydrocarbons	1
730	Pyrrolidines–Dioxanes	1
731	Pyrrolidines–Vinyl halides	1
732	Halohydrins–Allyl-type 1,3-dipolar organic compounds	1
733	Halohydrins–Organooxygen compounds	1
734	Piperidines–Tetrahydrofurans	1
735	Fatty Acyls–Oxanes	1
736	Piperidines–Organonitrogen compounds	1
737	Azolidines–Dioxanes	1
738	Organooxygen compounds–Phenol ethers	1
739	Oxathiolanes–NA	1
740	Unsaturated hydrocarbons–Oxazinanes	1
741	Unsaturated hydrocarbons–Carboximidic acids and derivatives	1
742	Fatty Acyls–Sulfoxides	1
743	Fatty Acyls–Organo-post-transition metal compounds	1
744	Fatty Acyls–Pyridines and derivatives	1
745	Organochlorides–Other non-metal organides	1

746	Lactones–Dioxanes	1
747	Benzene and substituted derivatives–Epoxides	1
748	Lactams–Polycyclic hydrocarbons	1
749	Alkyl halides–Fatty Acyls	1
750	Alkyl halides–Unsaturated hydrocarbons	1
751	Allyl-type 1,3-dipolar organic compounds–Homogeneous other non-metal compounds	1
752	Allyl-type 1,3-dipolar organic compounds–Organonitrogen compounds	1
753	Isoquinolines and derivatives–Benzene and substituted derivatives	1
754	Indenes and isoindenes–Benzene and substituted derivatives	1
755	Indenes and isoindenes–Unsaturated hydrocarbons	1
756	Lactams–Alkyl halides	1
757	Lactams–Organochlorides	1
758	Lactams–Organooxygen compounds	1
759	Alkyl halides–Phenols	1
760	Lactams–NA	1
761	Lactams–Dioxanes	1
762	Organofluorides–Allyl-type 1,3-dipolar organic compounds	1
763	Organofluorides–Dioxanes	1
764	Lactones–Tetrahydrofurans	1
765	Fatty Acyls–Prenol lipids	1
766	Saturated hydrocarbons–Oxanes	1
767	Saturated hydrocarbons–Epoxides	1
768	Saturated hydrocarbons–Organic disulfides	1
769	Alkyl halides–Other non-metal organides	1
770	Alkyl halides–Organobromides	1
771	Saturated hydrocarbons–Tetralins	1
772	Phenanthrenes and derivatives–Naphthalenes	1
773	Organic phosphoric acids and derivatives–Vinyl halides	1
774	Organic phosphoric acids and derivatives–Allyl-type 1,3-dipolar organic compounds	1
775	Phenols–Homogeneous other non-metal compounds	1
776	Phenols–Tetralins	1
777	Phenols–Organoiodides	1
778	Phenols–Organobromides	1
779	Phenols–Other non-metal organides	1
780	Phenols–Anthracenes	1
781	Phenols–Carboximidic acids and derivatives	1

782	Phenanthrenes and derivatives–Phenol ethers	1
783	Organooxygen compounds–Carboximidic acids and derivatives	1
784	Saturated hydrocarbons–Trialkylphosphites	1
785	Saturated hydrocarbons–Organic phosphoric acids and derivatives	1
786	Saturated hydrocarbons–Organic carbonic acids and derivatives	1
787	Organochlorides–Phenol ethers	1
788	Naphthalenes–Carboximidic acids and derivatives	1
789	Naphthalenes–Oxazinanes	1
790	Naphthalenes–Organoiodides	1
791	Naphthalenes–Organobromides	1
792	Naphthalenes–Dioxanes	1
793	Organoiodides–Organochlorides	1
794	Saturated hydrocarbons–Phenanthrenes and derivatives	1
795	Lactones–NA	1
796	NA–Heteroaromatic compounds	1
797	Stilbenes–Saturated hydrocarbons	1
798	Organochlorides–Pyridines and derivatives	1
799	Organobromides–Unsaturated hydrocarbons	1
800	Organochlorides–Organofluorides	1
801	Organofluorides–Prenol lipids	1
802	Organofluorides–Fatty Acyls	1
803	Organic oxoanionic compounds–Organooxygen compounds	1
804	Organic oxoanionic compounds–Organoiodides	1
805	Dioxolanes–Homogeneous other non-metal compounds	1
806	NA–Tetrahydrofurans	1
807	Organofluorides–Organochlorides	1
808	NA–Vinyl halides	1
809	NA–Dioxanes	1
810	Polycyclic hydrocarbons–NA	1
811	Polycyclic hydrocarbons–Benzene and substituted derivatives	1
812	Other non-metal organides–Homogeneous other non-metal compounds	1
813	Other non-metal organides–Allyl-type 1,3-dipolar organic compounds	1
814	Other non-metal organides–Organofluorides	1
815	Other non-metal organides–Dioxanes	1
816	Lactones–Allyl-type 1,3-dipolar organic compounds	1
817	Stilbenes–Unsaturated hydrocarbons	1

818	Organofluorides–Tetrahydrofurans	1
819	Saturated hydrocarbons–Anthracenes	1
820	Vinyl halides–NA	1
821	Tetrahydrofurans–Homogeneous other non-metal compounds	1
822	Tetrahydrofurans–Organo-post-transition metal compounds	1
823	Tetrahydrofurans–Allyl-type 1,3-dipolar organic compounds	1
824	Tetrahydrofurans–Organoiodides	1
825	Tetrahydrofurans–Organofluorides	1
826	Tetrahydrofurans–Organochlorides	1
827	Tetrahydrofurans–Organonitrogen compounds	1
828	Tetrahydrofurans–Fatty Acyls	1
829	Tetrahydrofurans–Dioxanes	1
830	Vinyl halides–Sulfoxides	1
831	Organobromides–Dioxanes	1
832	Vinyl halides–Pyridines and derivatives	1
833	Vinyl halides–Carboxylic acids and derivatives	1
834	Vinyl halides–Dioxanes	1
835	Naphthalenes–Heteroaromatic compounds	1
836	Naphthalenes–Tetrahydrofurans	1
837	Organonitrogen compounds–Fatty Acyls	1
838	Allyl-type 1,3-dipolar organic compounds–Dioxanes	1
839	Organobromides–Allyl-type 1,3-dipolar organic compounds	1
840	Organobromides–Organooxygen compounds	1
841	Homogeneous other non-metal compounds–Oxathiolanes	1

S9 Percentage of systems below absolute error in isothermal studies

Table S9: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 20°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	22.35	39.41	52.35
UNIFAC (Do)	45.88	65.88	75.88
COSMO-RS	30.59	50.00	64.71
MOSCED	**53.53**	**78.24**	**85.88**
GNNprevious	31.18	56.47	70.00
SolvGNN	51.76	70.59	82.94

Table S10: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 25°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	30.21	47.21	63.64
UNIFAC (Do)	40.47	61.88	73.02
COSMO-RS	27.27	48.39	62.17
MOSCED	47.51	69.50	80.65
GNNprevious	46.92	68.91	79.18
SolvGNN	**61.00**	**76.25**	**84.16**

Table S11: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 30°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	23.33	38.00	50.67
UNIFAC (Do)	32.67	53.33	68.00
COSMO-RS	24.00	46.00	60.00
MOSCED	**54.00**	**76.67**	**84.67**
GNNprevious	41.33	62.00	80.00
SolvGNN	42.00	70.67	79.33

Table S12: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 40°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	27.41	40.00	54.07
UNIFAC (Do)	27.41	52.59	65.93
COSMO-RS	21.48	41.48	62.22
MOSCED	45.19	66.67	72.59
GNNprevious	33.33	55.56	71.11
SolvGNN	**48.89**	**68.15**	**77.78**

Table S13: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 50°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	25.20	40.94	55.91
UNIFAC (Do)	40.16	56.69	71.65
COSMO-RS	24.41	43.31	59.84
MOSCED	49.61	73.23	**85.04**
GNNprevious	41.73	68.50	84.25
SolvGNN	**50.39**	**75.59**	82.68

Table S14: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 60°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	26.47	44.85	61.03
UNIFAC (Do)	36.03	59.56	70.59
COSMO-RS	28.68	47.06	62.50
MOSCED	**47.79**	68.38	82.35
GNNprevious	34.56	**72.06**	82.35
SolvGNN	45.59	71.32	**86.76**

Table S15: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 70°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	23.29	45.21	53.42
UNIFAC (Do)	36.99	65.75	**80.82**
COSMO-RS	27.40	38.36	60.27
MOSCED	49.32	65.75	76.71
GNNprevious	50.68	**72.60**	79.45
SolvGNN	**54.79**	69.86	76.71

Table S16: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 80°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	34.62	50.00	67.31
UNIFAC (Do)	46.15	65.38	80.77
COSMO-RS	28.85	40.38	51.92
MOSCED	46.15	61.54	73.08
GNNprevious	50.00	**82.69**	88.46
SolvGNN	**57.69**	**82.69**	**90.38**

Table S17: Percentage of systems in the test set that can be predicted by all models below the absolute error thresholds 0.1, 0.2 and 0.3 for temperature 100°C. RF refers to the random forest model. Higher is better, the best value per threshold is bold.

Method/AE	0.1	0.2	0.3
RF	18.60	30.23	34.88
UNIFAC (Do)	32.56	60.47	83.72
COSMO-RS	16.28	48.84	62.79
MOSCED	**39.53**	53.49	74.42
GNNprevious	37.21	**76.74**	**86.05**
SolvGNN	**39.53**	67.44	74.42

S10 Binary systems contained in the external dataset used for discrete extrapolation testing

Collection of all solvent-solute chemical classes contained in the external dataset used for testing the GH-GNN model for discrete extrapolation. If either the solute or solvent chemical class is missing, this indicates that that the class for such compound is "Not-available" according to Classyfire [1].

Table S18: Binary solvent-solute classes contained in the training set used for developing GH-GNN and their occurrences.

No.	Solvent-solute chemical classes	Systems
1	Fatty Acyls–Organooxygen compounds	147
2	Fatty Acyls–Saturated hydrocarbons	103
3	Organofluorides–Organooxygen compounds	96
4	Organonitrogen compounds–Benzene and substituted derivatives	93
5	Organonitrogen compounds–Organooxygen compounds	88
6	Fatty Acyls–Benzene and substituted derivatives	63
7	nan–Saturated hydrocarbons	60
8	Organooxygen compounds–Benzene and substituted derivatives	60
9	Organofluorides–Carboxylic acids and derivatives	48
10	Organooxygen compounds–Saturated hydrocarbons	48
11	nan–Benzene and substituted derivatives	42
12	Glycerolipids–Organooxygen compounds	41
13	Homogeneous other non-metal compounds–Organooxygen compounds	39
14	Organonitrogen compounds–Saturated hydrocarbons	39
15	Organonitrogen compounds–Unsaturated hydrocarbons	35
16	–Organooxygen compounds	34
17	Organofluorides–Unsaturated hydrocarbons	32
18	Fatty Acyls–Alkyl halides	32
19	Organofluorides–Benzene and substituted derivatives	32
20	Thiolanes–Saturated hydrocarbons	29
21	Glycerolipids–Benzene and substituted derivatives	29
22	Fatty Acyls–Organochlorides	29
23	Fatty Acyls–Unsaturated hydrocarbons	28
24	Organofluorides–Organonitrogen compounds	28
25	Organofluorides–Alkyl halides	27

26	Fatty Acyls–Carboxylic acids and derivatives	26
27	nan–Unsaturated hydrocarbons	24
28	nan–Organooxygen compounds	24
29	Glycerolipids–Saturated hydrocarbons	24
30	Organonitrogen compounds–Carboxylic acids and derivatives	23
31	Benzene and substituted derivatives–Saturated hydrocarbons	22
32	Saturated hydrocarbons–	22
33	Organic oxoanionic compounds–Saturated hydrocarbons	21
34	Fatty Acyls–Vinyl halides	20
35	–Saturated hydrocarbons	18
36	nan–Alkyl halides	18
37	–Benzene and substituted derivatives	16
38	Organofluorides–Allyl-type 1,3-dipolar organic compounds	16
39	Thiolanes–Benzene and substituted derivatives	14
40	Fatty Acyls–Phenol ethers	14
41	Benzene and substituted derivatives–Alkyl halides	12
42	Benzene and substituted derivatives–Carboxylic acids and derivatives	12
43	Organic disulfides–Saturated hydrocarbons	11
44	Unsaturated hydrocarbons–Unsaturated hydrocarbons	11
45	Homogeneous other non-metal compounds–Dioxolanes	10
46	Alkyl halides–Saturated hydrocarbons	10
47	Oxanes–	10
48	Homogeneous other non-metal compounds–Vinyl halides	10
49	Organonitrogen compounds–Organochlorides	10
50	Prenol lipids–	10
51	Organonitrogen compounds–Organonitrogen compounds	9
52	Homogeneous other non-metal compounds–Prenol lipids	9
53	Benzene and substituted derivatives–Organooxygen compounds	8
54	Prenol lipids–Organooxygen compounds	8
55	Organooxygen compounds–Organooxygen compounds	8
56	Homogeneous other non-metal compounds–Heteroaromatic compounds	8
57	Carboxylic acids and derivatives–Benzene and substituted derivatives	8
58	Organooxygen compounds–Unsaturated hydrocarbons	7
59	Polycyclic hydrocarbons–Unsaturated hydrocarbons	7
60	Carboxylic acids and derivatives–Unsaturated hydrocarbons	7
61	Benzene and substituted derivatives–Unsaturated hydrocarbons	7

62	Saturated hydrocarbons–Unsaturated hydrocarbons	7
63	Organonitrogen compounds–Alkyl halides	7
64	Benzene and substituted derivatives–Vinyl halides	6
65	Carboxylic acids and derivatives–Saturated hydrocarbons	6
66	Glycerolipids–Vinyl halides	6
67	Glycerolipids–Alkyl halides	6
68	Glycerolipids–Phenol ethers	6
69	nan–Carboxylic acids and derivatives	6
70	Glycerolipids–Unsaturated hydrocarbons	6
71	Organooxygen compounds–Alkyl halides	6
72	nan–Organonitrogen compounds	6
73	Glycerolipids–Carboxylic acids and derivatives	6
74	Unsaturated hydrocarbons–Benzene and substituted derivatives	6
75	Oxazinanes–Saturated hydrocarbons	6
76	Organic oxoanionic compounds–Benzene and substituted derivatives	6
77	Saturated hydrocarbons–Saturated hydrocarbons	5
78	Oxanes–Saturated hydrocarbons	5
79	Oxazinanes–	5
80	–Carboxylic acids and derivatives	5
81	Prenol lipids–Saturated hydrocarbons	5
82	Polycyclic hydrocarbons–Saturated hydrocarbons	5
83	–Organochlorides	4
84	Unsaturated hydrocarbons–Saturated hydrocarbons	4
85	Fatty Acyls–Tetrahydrofurans	4
86	Sulfoxides–Unsaturated hydrocarbons	4
87	Fatty Acyls–Organonitrogen compounds	4
88	Carboxylic acids and derivatives–Organooxygen compounds	4
89	–Alkyl halides	4
90	Glycerolipids–Organochlorides	4
91	Benzene and substituted derivatives–	4
92	Prenol lipids–Carboxylic acids and derivatives	4
93	Alkyl halides–Benzene and substituted derivatives	4
94	–Vinyl halides	4
95	–Phenol ethers	4
96	Organic disulfides–Benzene and substituted derivatives	3
97	Dihydrothiophenes–Benzene and substituted derivatives	3

98	Pyrrolidines–Unsaturated hydrocarbons	3
99	Organooxygen compounds–nan	3
100	Organooxygen compounds–Organochlorides	3
101	Dihydrothiophenes–Saturated hydrocarbons	3
102	Glycerolipids–	3
103	Prenol lipids–Vinyl halides	3
104	–Unsaturated hydrocarbons	3
105	Organooxygen compounds–Carboxylic acids and derivatives	3
106	Saturated hydrocarbons–Vinyl halides	3
107	Saturated hydrocarbons–Organooxygen compounds	2
108	Carboxylic acids and derivatives–Alkyl halides	2
109	Unsaturated hydrocarbons–Phenol ethers	2
110	Thiolanes–Unsaturated hydrocarbons	2
111	Organooxygen compounds–Dioxanes	2
112	Organooxygen compounds–Organonitrogen compounds	2
113	Unsaturated hydrocarbons–Organooxygen compounds	2
114	Organooxygen compounds–Tetrahydrofurans	2
115	Prenol lipids–Organonitrogen compounds	2
116	Oxathianes–Unsaturated hydrocarbons	2
117	Carboxylic acids and derivatives–Organochlorides	2
118	Polycyclic hydrocarbons–nan	2
119	Prenol lipids–Benzene and substituted derivatives	1
120	Prenol lipids–Allyl-type 1,3-dipolar organic compounds	1
121	Homogeneous other non-metal compounds–Trioxanes	1
122	Polycyclic hydrocarbons–Benzene and substituted derivatives	1
123	Prenol lipids–Organic carbonic acids and derivatives	1
124	Prenol lipids–Organic phosphoric acids and derivatives	1
125	Prenol lipids–Sulfoxides	1
126	Prenol lipids–Organochlorides	1
127	Homogeneous other non-metal compounds–	1
128	Prenol lipids–Other non-metal organides	1
129	Prenol lipids–Unsaturated hydrocarbons	1
130	Carboxylic acids and derivatives–Tetrahydrofurans	1
131	Carboxylic acids and derivatives–Allyl-type 1,3-dipolar organic compounds	1
132	–Organonitrogen compounds	1
133	Carboxylic acids and derivatives–Carboxylic acids and derivatives	1

134	Sulfonyls–Unsaturated hydrocarbons	1
135	Carboxylic acids and derivatives–nan	1
136	Carboximidic acids and derivatives–Unsaturated hydrocarbons	1
137	Carboxylic acids and derivatives–Organobromides	1
138	Carboxylic acids and derivatives–Organonitrogen compounds	1
139	Carboxylic acids and derivatives–Dioxanes	1
140	Unsaturated hydrocarbons–	1
141	Phenol esters–Saturated hydrocarbons	1
142	Organonitrogen compounds–Dioxanes	1
143	Organonitrogen compounds–Allyl-type 1,3-dipolar organic compounds	1
144	Organonitrogen compounds–Phenol ethers	1
145	Organonitrogen compounds–Tetrahydrofurans	1
146	Organonitrogen compounds–Fatty Acyls	1
147	Organonitrogen compounds–Phenols	1
148	Organonitrogen compounds–Pyridines and derivatives	1
149	Homogeneous other non-metal compounds–Benzene and substituted derivatives	1

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