Supplementary Information (SI) for Journal of Materials Chemistry C.

An Integrated High-Throughput Screening Framework for Perovskite Light-Emitting Diodes Passivators Based on Machine Learning

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1 ML Methods

1.1 Descriptor Selection and Value Extraction

Implementation workflow:

The overall workflow consists of the following steps:

(1) SMILES acquisition: The SMILES representations of passivator molecules are collected manually from literatures (training data) or Pubchem (predicition data).

(2) Molecular parsing with RDKit: Each SMILES string is converted into an RDKit Mol object by coding (e.g. Displaying hydrogen atoms), which serves as the basis for all subsequent descriptor calculations.

(3) Descriptor definition and customization: A predefined list of RDKit molecular descriptors is specified, covering physicochemical properties, structural features, and hydrogen-bond-related parameters. In addition, custom descriptors (e.g., halogen atom counts) are implemented via user-defined functions to capture chemically relevant features that are not directly available in standard RDKit descriptors.

(4) Automated feature extraction: An iterative loop is used to compute all descriptor values for each molecule and automatically insert them into the corresponding columns of the dataset.

(5) Data output and extensibility: The resulting descriptor matrix is exported in a structured format and can be readily extended to include additional descriptors or applied to new molecular systems without modifying the overall pipeline logic. The workflow is implemented in the open-source code with a notebook version (1.Collecting_data_desr_w.ipynb), and the detailed key scripts has also been given as follows:

```
'''
#Part 1
#Define halide atom calculator funtion
def Halide_accumulator(mol):
    Num_Fluorine_atoms = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 9)#F
    Num_Chlorine_Atoms = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 17)#Cl
    Num_Bromine_Atoms = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 35)#Br
    Num_Iodine_atoms = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 53)#I
    Num_Halide_Atoms =  Num_Fluorine_atoms + Num_Chlorine_Atoms +Num_Bromine_Atoms +  Num_Iodine_atoms
return Num_Halide_Atoms
#Part 2
#Create a sheet of descriptors
smi = data_set['IsomericSMILES'].to_list()
feature_columns = [
    'Heavy_atoms',
    'H_Acceptors',
    'H_Donors',
    'Rot_bonds',
```

```
    'Val_electrons',
    'Mol_Wt',
    'Topo',
    'TPSA',
    'AvgIpc',
    'Carbon',
    'Hydrogen',
    'Oxide',
    'Nitrogen',
    'Halide'
]
#Set the default value as null
for col in feature_columns:
    data_set[col] = ' '
print(f"shape:{data_set.shape}")
data_set = data_set.iloc[:,:]
#Part 3
#Loop through and write
for i in range(len(smi)):
    mol_hided_H = Chem.MolFromSmiles(smi[i])
    #Display hydrogen atoms
    mol = Chem.AddHs(mol_hided_H)
    #The number of Heavy atoms a molecule
    data_set.loc[i,'Heavy_atoms'] = Lipinski.HeavyAtomCount(mol)
    #The number of Hydrogen Bond Acceptors
    data_set.loc[i,'H_Acceptors'] = Lipinski.NumHAcceptors(mol)
    #The number of Hydrogen Bond Donors
    data_set.loc[i,'H_Donors'] = Lipinski.NumHDonors(mol)

    #The number of Rotatable Bonds
    data_set.loc[i,'Rot_bonds'] = Lipinski.NumRotatableBonds(mol)
    #The number of Valence Electrons
    data_set.loc[i,'Val_electrons'] = Descriptors.NumValenceElectrons(mol)
    #The average molecular Weight of the molecule, g/mol
    data_set.loc[i,'Mol_Wt'] = Descriptors.MolWt(mol)
    #The topological index, which quantifies “complexity” of molecules
    data_set.loc[i,'Topo'] = GraphDescriptors.BertzCT(mol)
    #The topological molecular polar surface area
    data_set.loc[i,'TPSA'] = Descriptors.TPSA(mol)
    #The average information content of the coefficients of the characteristic polynomial of the adjacency matrix of a hydrogen-suppressed graph of a molecule
    data_set.loc[i,'AvgIpc'] = GraphDescriptors.AvgIpc(mol)
    #The number of carbon, hydrogen, nitrogen, oxygen and Halide atoms
```

```
    data_set.loc[i,'Carbon'] = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 6)#C
    data_set.loc[i,'Hydrogen'] = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 1)#H
    data_set.loc[i,'Oxide'] = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 8)#O
    data_set.loc[i,'Nitrogen'] = sum(1 for atom in mol.GetAtoms() if atom.GetAtomicNum() == 7)#N
    data_set.loc[i,'Halide'] = Halide_accumulator(mol)#Cl Br I
dataset_add_features = data_set.iloc[:len(smi),:]
#Select samples with a target below 5.0
dataset_add_features = dataset_add_features[dataset_add_features['EQE enhanced ratio'] <= 5.0]

#One-hot encoder
from sklearn.preprocessing import OneHotEncoder
encoder = OneHotEncoder(sparse_output=False)
dataset_add_features['A_site'] = encoder.fit_transform(dataset_add_features[['A_site']])
print(f"shape:{dataset_add_features.shape}")
dataset_add_features.to_csv("data/dataset_with_features.csv",index=False)
'''
```

1.2 Data Collection and Preprocessing

A comprehensive literature survey was conducted covering publications from the past decade using the keyword “Green Perovskite LED Passivation”. Relevant studies were manually screened, and key information required for machine learning tasks was extracted, including the passivator name, PeLEDs device components, A-site type, control external quantum efficiencies (EQEs), passivated EQEs, as well as article titles and DOIs. All collected data are summarized in Supplementary Information Data 1. To improve data reliability and reduce potential bias, data points with an EQE enhancement ratio greater than 5 were excluded from the dataset. Early-stage studies often reported extremely low initial EQEs due to limitations in fabrication processes, which could result in disproportionately large enhancement ratios after passivation. Such values are not representative of current experimental practices and may adversely affect model training. After data preprocessing, the same curated dataset was used for training and optimizing all machine learning models. This ensured consistency across different models and enabled a fair comparison of their predictive performance, facilitating the identification of the most suitable machine learning model for this study.

1.3 Hyperparameter optimization

Hyperparameter optimization was performed exclusively during the model training stage to improve predictive performance and generalization ability. For each machine learning model, an initial parameter range was defined based on prior experience and preliminary tests. Hyperparameters were then optimized using a grid search strategy combined with five-fold cross-validation. During this process, model performance was evaluated iteratively across different hyperparameter combinations, and the average cross-validation score was used as the selection criterion. Manual tuning was further applied to refine key hyperparameters around the optimal regions identified by grid search. This combined strategy ensured efficient exploration of the parameter space while avoiding overfitting. The final optimized hyperparameter sets for all models are summarized in the following Table, and the corresponding implementation details are provided in the open-source code repository.

Taking the hyper-parameter optimization for CatBoost model as an example:

```
'''
from catboost import CatBoostRegressor
```

```
cat_reg = CatBoostRegressor(learning_rate= 0.25 ,bagging_temperature= 1,verbose = 0 ,random_state=42)
param_grid = {
   'iterations': [400,410,420],
   'depth': [5,10],
}
search = GridSearchCV(cat_reg, param_grid, cv = 5,n_jobs = -1,error_score = 'raise',verbose = 0)
search.fit(X_train, y_train)
print(f'cat_reg best parameters: {search.best_params_}')
best_catreg = search.best_estimator_
'''
```

1.4 Criteria for the passivation candidates

Based on model interpretation analysis, several molecular features were identified as key contributors to passivation effectiveness. In particular, the model indicated that favorable passivators for PeLEDs typically possess a hydrogen bond donor (HBD) count greater than one and a molecular weight below approximately 300 g/mol, which informed the initial screening criteria.

On this basis, the prediction set was constructed according to the following principles:

(a) Consistency with model-derived criteria: Candidate molecules were required to satisfy the key descriptors identified from model interpretation, specifically an HBD count greater than one and a molecular weight of approximately below 300 g/mol.

(b) Inclusion of chemically relevant functional groups: Molecules containing functional groups known to interact with perovskite defects were preferentially selected, including ammonium, hydroxyl, carbonyl, nitro, phosphoryl, and sulfonic acid moieties.

(c) Structural similarity to known passivators: To ensure chemical plausibility and extrapolation reliability, candidates were chosen to exhibit structural resemblance to passivators in the training set, considering factors such as molecular symmetry, aromatic ring distribution, and overall molecular topology.

By integrating model interpretability, chemical intuition, and structural similarity considerations, this design strategy ensures that the prediction set is both chemically meaningful and aligned with the learned structure–property relationships, thereby increasing the likelihood of identifying effective passivation molecules.

2. Results of ML

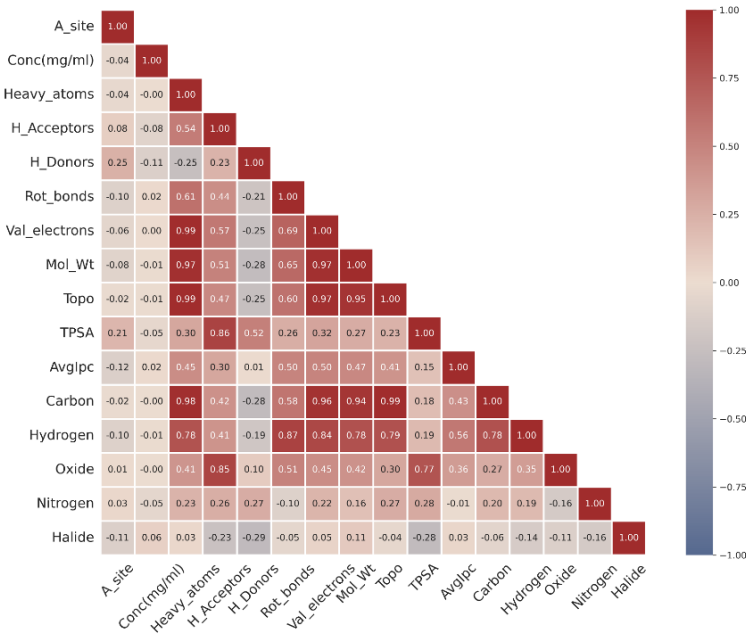

Fig. S1. Heatmap of Pearson product-moment correlation coefficient of initial features.

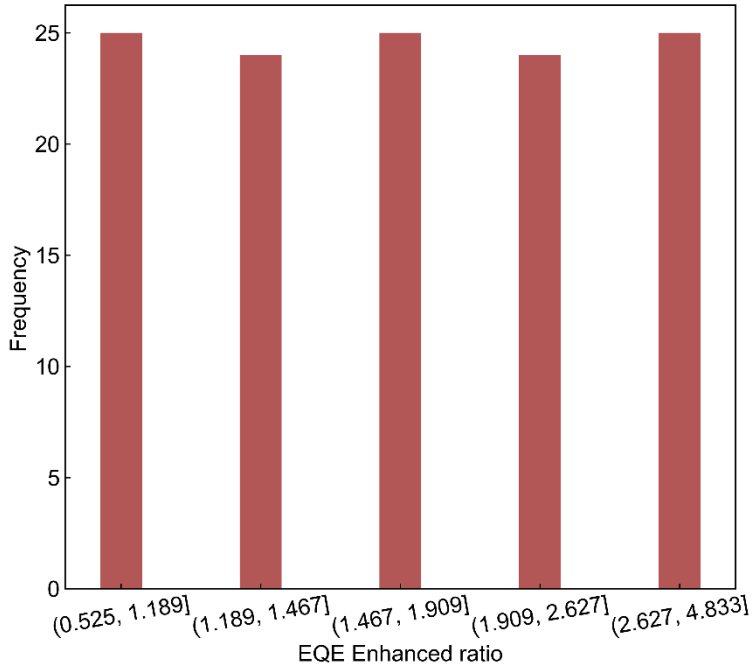

Fig. S2. Quintile-based analysis of samples.

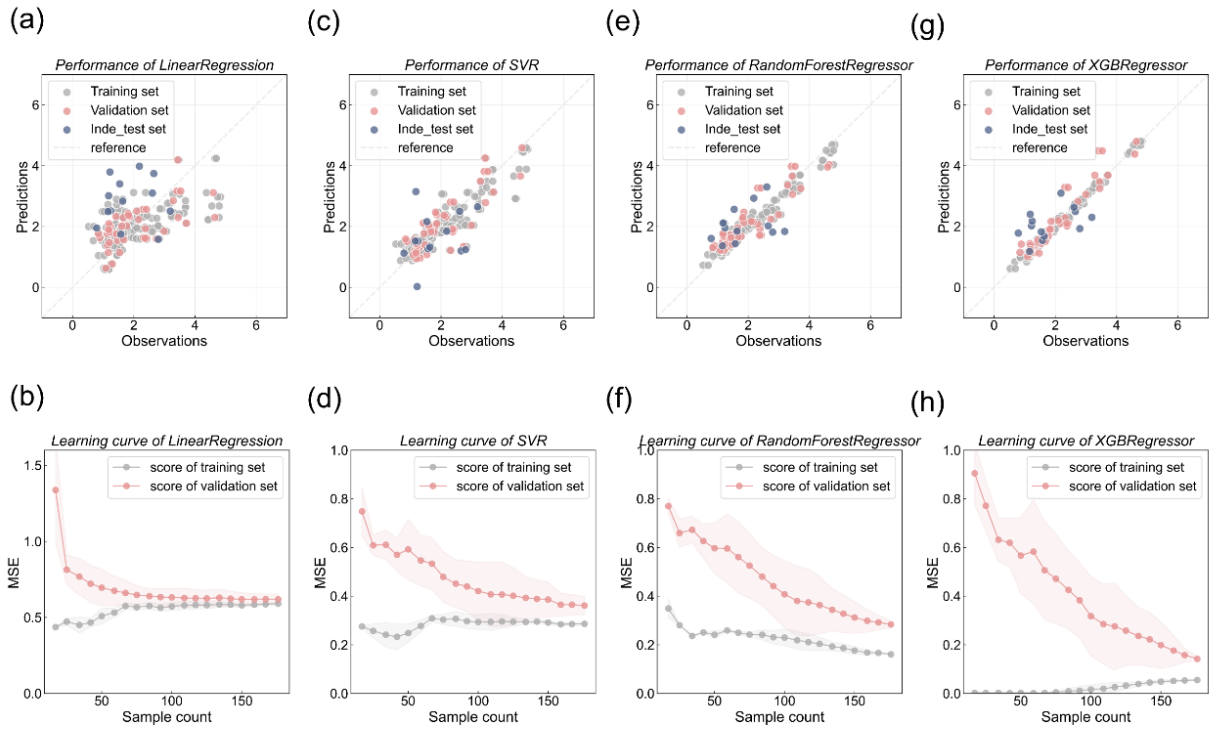

Fig. S3. The remain models' performance. a), c), e), g). Predictions and observations for the LR, SVR, RF, and XGBoost, respectively. b), d), f), g) The learning curves for the LR, SVR, RF, and XGBoost, respectively.

Table S1. The optimized hyperparameters for models

Model	Hyperparameter key and value
LR	fit_intercept=True, copy_X=True, n_jobs=None, positive=False
SVR	C = 15, epsilon = 0.2
RF	max_depth = 10, min_samples_leaf'=1, min_samples_split:=2, n_estimators =80, random_state = 42
XGBoost	subsample = 0.8,objective='reg:squarederror',random_state = 42, max_depth = 10, min_child_weight = 3, n_estimators =125
CatBoost	Depth = 5, iterations = 410,learning_rate= 0.25 ,bagging_temperature= 1,verbose = 0 ,random_state=42

Table S2. The CIDs of 70 molecules from PubChem as the candidates for prediction

CID	CID	CID	CID	CID	CID	CID
7812	222556	5570	8431	30209	12495	255
7423	28159	72924	9808	9395	7873	12793
9731	379	936	160117	7416	31357	6327654
7447	612	240	1176	1678	13134	74188
7441	978	69150	20861	1493	668	6327349
79617	370	75498	120047	5955	6535	78452
11118	1066	7487	980	7475	9275	7369
75655	967	68400	12307	8330	654	985
74218	3845	26323	16782	7430	1015	12669616
136315	3442	54747	62823	7492	14017	4190003

3. DFT Validation

DFT calculations: Ab-initio calculations were performed using the Vienna Ab-initio Simulation Package (VASP) code with the projector augmented wave method (PAW).[1-4] The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) was chosen for electron exchange and correlation.[5] The criteria of energy/force convergence and energy cutoff were set at 10−4 eV/0.05 eV Å−1 and 400 eV, respectively. We utilized Monkhorst-Pack scheme with 2×2×1 k-point grid to calculate $CsPbBr_3$ surfaces with/without defects and the passivated models with 5 different representative molecules, respectively. In more detail, a 3×3×4 supercell crystal was generated by expanding the $CsPbBr_3$ primitive cell. An 18 Å vacuum layer was inserted above the adsorption surface, and a Br vacancy (V_{Br}) defect was constructed on the crystal surface. Both the initial state of the molecule-passivated crystal and the small molecules were in their relaxed lowest-energy configurations after relaxation calculations. All crystal structures were constructed by *Materials Studio* and *Vesta.*

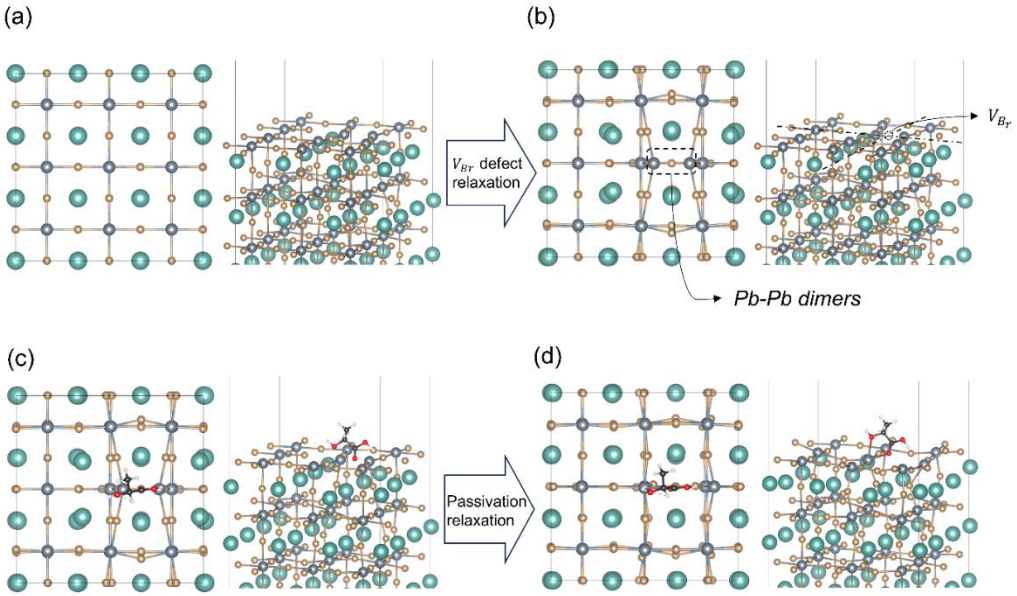

Fig. S4. Top-view and 45-degree front-view illustrations of the $CsPbBr_3$ passivation process with 2-HPA. a) Pristine slab without surface defects， b) The slab with a V_{Br} defect, where Pb-Pb dimers formed after relaxation, c) Initial situation of 2-HPA adsorbed on the surface, d) After 2-HPA passivated the V_{Br} defect, the Pb-Pb dimers disappeared.

Table S3. Adsorption energy results of five passivation molecules used for DFT theoretical validation.

Passivator	E_{pass} [eV]	E_{slab} [eV]	$E_{pass/slab}$ [eV]	E_{ads} [eV]
2-HPA	-69.55	-510.29	-580.12	-0.28
P-3-CA	-99.42	-510.29	-609.98	-0.27
DHP	-78.35	-510.29	-589.18	-0.54
BS0C	-91.59	-510.29	-604.85	-2.97
1,2,4,5-TE-3-NB	-84.54	-510.29	-597.02	-2.19

$$E_{ads} = E_{pass/slab} - E_{slab} - E_{pass}$$

where $E_{pass/slab}$ is the energy of the passivator-adsorbed system, E_{slab} is the energy of defective surface slab and E_{pass} is the energy of passivator(molecule). The negative adsorption energies of all systems show that passivator could be stably adsorbed on the surface with defects.

References

1. J. P. Perdew, *Physical review B*, 1986, **33**, 8822.
2. G. Kresse and J. Furthmüller, *Physical review B*, 1996, **54**, 11169.
3. G. Kresse and D. Joubert, *Physical review b*, 1999, **59**, 1758.
4. J. P. Perdew, K. Burke and M. Ernzerhof, *Physical review letters*, 1996, **77**, 3865.
5. J. P. Perdew, K. Burke and M. Ernzerhof, *Physical Review Letters*, 1998, **80**, 891.

Green Perovskite Light Emitting Diodes from Literature

Number	PeLEDs component	PA	IsomericSMILES	A_site	Conc(mg/ml)	Control device EQE	Passivated device EQE	EQE enhanced ratio	article title	Doi	Emitting Layer structure	year
1	PPA2FAn−1PbnBr3n+1	trimorpholinophosphine oxide	C1COCCN1P(=O)(N2CCOCC2)N3CCOCC3	organic	2.000	2.79%	4.40%	1.5771	Improving Green Perovskite Nanoplate Light-Emitting Diode Performance via Precision Passivation and Phase Distribution Management	https://doi.org/10.1021/acsanm.3c06224	quasi-2D	2024
1	PPA2FAn−1PbnBr3n+1	trimorpholinophosphine oxide	C1COCCN1P(=O)(N2CCOCC2)N3CCOCC3	organic	6.000	2.79%	5.85%	2.0968	Improving Green Perovskite Nanoplate Light-Emitting Diode Performance via Precision Passivation and Phase Distribution Management	https://doi.org/10.1021/acsanm.3c06224	quasi-2D	2024
1	PPA2FAn−1PbnBr3n+1	trimorpholinophosphine oxide	C1COCCN1P(=O)(N2CCOCC2)N3CCOCC3	organic	4.000	2.79%	7.31%	2.6201	Improving Green Perovskite Nanoplate Light-Emitting Diode Performance via Precision Passivation and Phase Distribution Management	https://doi.org/10.1021/acsanm.3c06224	quasi-2D	2024
2	CsPbBr3	Lithium bromide	[Li+].[Br-]	inorganic	1.738	2.83%	7.92%	2.7986	High-Performance Perovskite Light-Emitting Diode with Enhanced Operational Stability Using Lithium Halide Passivation	https://doi.org/10.1002/anie.201914000	3D	2019
2	CsPbBr3	Lithium bromide	[Li+].[Br-]	inorganic	3.476	2.83%	16.20%	5.7244	High-Performance Perovskite Light-Emitting Diode with Enhanced Operational Stability Using Lithium Halide Passivation	https://doi.org/10.1002/anie.201914000	3D	2019
3	PEA2PbBr4(CsPbBr3)4	ethoxylated trimethylolpropane triacrylate	CCC(COCCOC(=O)C=C)(COCCOC(=O)C=C)COCCOC(=O)C=C	inorganic	5.000	16.79%	22.49%	1.3395	Perovskite Light-Emitting Diodes with External Quantum Efficiency Exceeding 22% via Small-Molecule Passivation	https://doi.org/10.1002/adma.202007169	quasi-2D	2021
4	PEA2(FAPbBr3)n-1PbBr4 (n=3)	trioctylphosphine oxide	CCCCCCCCP(=O)(CCCCCCCC)CCCCCCCC	organic	2.000	10.00%	14.36%	1.4360	Efficient green light-emitting diodes based on quasi-two-dimensional composition and phase engineered perovskite with surface passivation	https://www.nature.com/articles/s41467-018-02978-7	quasi-2D	2018
5	PEA:CsPbBr3	methylene-bis-acrylamide	C=CC(=O)NCNC(=O)C=C	inorganic	4.625	11.30%	16.80%	1.4867	Green Perovskite Light-Emitting Diodes with 200 Hours Stability and 16% Efficiency: Cross-Linking Strategy and Mechanism	https://doi.org/10.1002/adfm.202011003	quasi-2D	2020
6	PEA:CsPbBr3	ammonium thiocyanate	C(#N)[S-].[NH4+]	inorganic	4.000	3.20%	10.50%	3.2813	Interface engineering improves the performance of green perovskite light-emitting diodes	https://doi.org/10.1039/D1TC05706E	quasi-2D	2022
6	PEA:CsPbBr3	ammonium thiocyanate	C(#N)[S-].[NH4+]	inorganic	8.000	3.20%	11.30%	3.5313	Interface engineering improves the performance of green perovskite light-emitting diodes	https://doi.org/10.1039/D1TC05706E	quasi-2D	2022
6	PEA:CsPbBr3	ammonium thiocyanate	C(#N)[S-].[NH4+]	inorganic	6.000	3.20%	14.70%	4.5938	Interface engineering improves the performance of green perovskite light-emitting diodes	https://doi.org/10.1039/D1TC05706E	quasi-2D	2022
7	DDA0.75HDA0.25Cs3Pb4Br13	diphenyl-4-triphenylsilylphenyl phosphine oxide	C1=CC=C(C=C1)[Si](C2=CC=CC=C2)(C3=CC=CC=C3)C4=CC=C(C=C4)P(=O)(C5=CC=CC=C5)C6=CC=CC=C6	inorganic	1.000	10.90%	11.90%	1.0917	Effect of Passivating Molecules and Antisolvents on Lifetime of Green Dion–Jacobson Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acsami.3c02170	quasi-2D DJ	2023
7	DDA0.75HDA0.25Cs3Pb4Br13	triphenylphosphine oxide	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC=C3	inorganic	1.000	10.90%	12.40%	1.1376	Effect of Passivating Molecules and Antisolvents on Lifetime of Green Dion–Jacobson Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acsami.3c02170	quasi-2D DJ	2023
7	DDA0.75HDA0.25Cs3Pb4Br13	triphenylphosphine oxide	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC=C3	inorganic	0.500	10.90%	12.70%	1.1651	Effect of Passivating Molecules and Antisolvents on Lifetime of Green Dion–Jacobson Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acsami.3c02170	quasi-2D DJ	2023
8	PEA2Csn–1PbnBr3n+1	Orthosilicic acid	O[Si](O)(O)O	inorganic		14.00%	16.60%	1.1857	In-situ passivation perovskite targeting efficient light-emitting diodes via spontaneously formed silica network	https://doi.org/10.1016/j.nanoen.2020.105134	quasi-2D	2020
9	CsPbBr3	(4-diphenylphosphorylphenyl)-triphenylsilane	C1=CC=C(C=C1)[Si](C2=CC=CC=C2)(C3=CC=CC=C3)C4=CC=C(C=C4)P(=O)(C5=CC=CC=C5)C6=CC=CC=C6	inorganic		7.70%	18.70%	2.4286	A bilateral interfacial passivation strategy promoting efficiency and stability of perovskite quantum dot light-emitting diodes	https://www.nature.com/articles/s41467-020-17633-3	qutatum dots	2020
10	PEA:CsPbBr3	Poly(vinylidene fluoride) (PVDF)	C=C(F)F	inorganic	0.050	15.10%	17.80%	1.1788	Polymer-Assisted Crystal Growth Regulation and Defect Passivation for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202203371	quasi-2D	2022
10	PEA:CsPbBr3	Poly(vinylidene fluoride) (PVDF)	C=C(F)F	inorganic	1.000	15.10%	18.10%	1.1987	Polymer-Assisted Crystal Growth Regulation and Defect Passivation for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202203371	quasi-2D	2022
10	PEA:CsPbBr3	Poly(vinylidene fluoride) (PVDF)	C=C(F)F	inorganic	5.000	15.10%	18.80%	1.2450	Polymer-Assisted Crystal Growth Regulation and Defect Passivation for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202203371	quasi-2D	2022
10	PEA:CsPbBr3	Poly(vinylidene fluoride) (PVDF)	C=C(F)F	inorganic	4.000	15.10%	19.30%	1.2781	Polymer-Assisted Crystal Growth Regulation and Defect Passivation for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202203371	quasi-2D	2022
10	PEA:CsPbBr3	Poly(vinylidene fluoride) (PVDF)	C=C(F)F	inorganic	2.000	15.10%	19.70%	1.3046	Polymer-Assisted Crystal Growth Regulation and Defect Passivation for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202203371	quasi-2D	2022
10	PEA:CsPbBr3	Poly(vinylidene fluoride) (PVDF)	C=C(F)F	inorganic	3.000	15.10%	22.29%	1.4762	Polymer-Assisted Crystal Growth Regulation and Defect Passivation for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202203371	quasi-2D	2022
11	CsPbBr3:PMMA	poly (arylonitrile)	C=CC#N	inorganic		6.90%	12.80%	1.8551	Multifunctional TADF Additives for High-Performance Green Perovskite Light-Emitting DiodesClick to copy article link	https://doi.org/10.1016/j.cej.2022.139927	3D	2022
12	PEA2FAn-1PbnBr3n+1(n=5)	2,7-dibromo-9,9-bis (3'-diethoxylphosphorylpropyl)-fluorene	CCOP(=O)(CCCC1(C2=C(C=CC(=C2)Br)C3=C1C=C(C=C3)	organic	2.041	18.10%	19.80%	1.0939	Suppressing thermal quenching via defect passivation for efficient quasi-2D perovskite light-emitting diodes	https://www.nature.com/articles/s41377-022-00761-4	quasi-2D	2022
12	PEA2FAn-1PbnBr3n+1(n=5)	2,7-dibromo-9,9-bis (3'-diethoxylphosphorylpropyl)-fluorene	CCOP(=O)(CCCC1(C2=C(C=CC(=C2)Br)C3=C1C=C(C=C3)	organic	1.020	18.10%	21.00%	1.1602	Suppressing thermal quenching via defect passivation for efficient quasi-2D perovskite light-emitting diodes	https://www.nature.com/articles/s41377-022-00761-4	quasi-2D	2022
12	PEA2FAn-1PbnBr3n+1(n=5)	2,7-dibromo-9,9-bis (3'-diethoxylphosphorylpropyl)-fluorene	CCOP(=O)(CCCC1(C2=C(C=CC(=C2)Br)C3=C1C=C(C=C3)	organic	0.340	18.10%	21.10%	1.1657	Suppressing thermal quenching via defect passivation for efficient quasi-2D perovskite light-emitting diodes	https://www.nature.com/articles/s41377-022-00761-4	quasi-2D	2022
12	PEA2FAn-1PbnBr3n+1(n=5)	2,7-dibromo-9,9-bis (3'-diethoxylphosphorylpropyl)-fluorene	CCOP(=O)(CCCC1(C2=C(C=CC(=C2)Br)C3=C1C=C(C=C3)	organic	0.680	18.10%	21.50%	1.1878	Suppressing thermal quenching via defect passivation for efficient quasi-2D perovskite light-emitting diodes	https://www.nature.com/articles/s41377-022-00761-4	quasi-2D	2022
13	CsPbBr3	poly(vinyl pyrrolidone) (PVP)	C=CN1CCCC1=O	inorganic	4.000	9.18%	17.09%	1.8617	Improving Perovskite Green Quantum Dot Light-Emitting Diode Performance by Hole Interface Buffer Layers	https://doi.org/10.1021/acsami.3c04592	qutatum dots	2023
13	CsPbBr3	poly(methyl methacrylate) (PMMA)	CC(=C)C(=O)OC	inorganic	0.500	9.18%	20.71%	2.2560	Improving Perovskite Green Quantum Dot Light-Emitting Diode Performance by Hole Interface Buffer Layers	https://doi.org/10.1021/acsami.3c04592	qutatum dots	2023
14	PEA2PbBr4(FAPbBr3)4	trimethylolpropane trimethacrylate	CCC(COC(=O)C(=C)C)(COC(=O)C(=C)C)COC(=O)C(=C)C	organic	0.677	17.70%	18.10%	1.0226	Engineering of Annealing and Surface Passivation toward Efficient and Stable Quasi-2D Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acs.jpclett.1c03413	quasi-2D	2021
14	PEA2PbBr4(FAPbBr3)4	trimethylolpropane trimethacrylate	CCC(COC(=O)C(=C)C)(COC(=O)C(=C)C)COC(=O)C(=C)C	organic	0.677	15.70%	18.20%	1.1592	Engineering of Annealing and Surface Passivation toward Efficient and Stable Quasi-2D Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acs.jpclett.1c03413	quasi-2D	2021
15	CsPbBr3	potassium thiocyanate	C(#N)[S-].[K+]	inorganic	2.000	5.80%	13.80%	2.3793	The efficient green light-emitting diodes based on low-toxicity Zr-Pb alloy perovskite quantum dots passivated by inorganic ligand	https://doi.org/10.1016/j.apmt.2022.101658	qutatum dots	2022
16	CsPbBr3	tributylphosphine oxide	CCCCP(=O)(CCCC)CCCC	inorganic	0.041	3.00%	9.98%	3.3267	High Color Purity and Efficient Green Light-Emitting Diode Using Perovskite Nanocrystals with the Size Overly Exceeding Bohr Exciton	https://doi.org/10.1021/jacs.1c09948	3D	2021
17	CsPbBr3	Guanidine bromide	NC(N)=N.[H]Br	inorganic	3.474	6.98%	10.06%	1.4413	Achieving high-efficiency CsPbBr3 perovskite light emitting diode via GABr- didecyldimethyl ammonium bromide hybrid ligand passivation	https://doi.org/10.1016/j.orgel.2023.106797	qutatum dots	2023
18	FAPbBr3/PEA2PbBr4	phenethylammonium bromide	C1=CC=C(C=C1)CCN.Br	organic	3.000	4.60%	9.00%	1.9565	Bifacial passivation towards efficient FAPbBr3-based inverted perovskite light-emitting diode	https://doi.org/10.1039/D0NR02323J	3D/2D	2020
19	MAPbBr3	ethylenediamine	C(CN)N	organic		0.12%	0.58%	4.8333	Amine-Based Passivating Materials for Enhanced Optical Properties and Performance of Organic–Inorganic Perovskites in Light-Emitting Diodes	https://doi.org/10.1021/acs.jpclett.7b00372	3D	2017
20	MAPbBr3	diphenyl chlorophosphite	C1=CC=C(C=C1)OP(OC2=CC=CC=C2)Cl	organic	16.421	12.80%	16.20%	1.2656	Phase Regulation and Defect Passivation Enabled by Phosphoryl Chloride Molecules for Efficient Quasi-2D Perovskite Light-Emitting	https://link.springer.com/article/10.1007/s40820-023-01089-3	quasi-2D	2023
20	MAPbBr3	bis(dimethylamino)phosphoryl chloride	CN(C)P(=O)(N(C)C)Cl	organic	5.970	12.80%	16.50%	1.2891	Phase Regulation and Defect Passivation Enabled by Phosphoryl Chloride Molecules for Efficient Quasi-2D Perovskite Light-Emitting	https://link.springer.com/article/10.1007/s40820-023-01089-3	quasi-2D	2023
20	MAPbBr3	dimethyl chlorophosphate	COP(=O)(OC)Cl	organic	7.225	12.80%	17.20%	1.3438	Phase Regulation and Defect Passivation Enabled by Phosphoryl Chloride Molecules for Efficient Quasi-2D Perovskite Light-Emitting	https://link.springer.com/article/10.1007/s40820-023-01089-3	quasi-2D	2023
20	MAPbBr3	diphenylphosphinic chloride	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)Cl	organic	19.772	12.80%	18.00%	1.4063	Phase Regulation and Defect Passivation Enabled by Phosphoryl Chloride Molecules for Efficient Quasi-2D Perovskite Light-Emitting	https://link.springer.com/article/10.1007/s40820-023-01089-3	quasi-2D	2023
20	MAPbBr3	bis(2-oxo-3-oxazolidinyl) phosphinic chloride	ClP(=O)(N1CCOC1=O)N2CCOC2=O	organic	6.364	12.80%	20.82%	1.6266	Phase Regulation and Defect Passivation Enabled by Phosphoryl Chloride Molecules for Efficient Quasi-2D Perovskite Light-Emitting	https://link.springer.com/article/10.1007/s40820-023-01089-3	quasi-2D	2023
21	MAPbBr3	4-aminobenzonitrile	C1=CC(=CC=C1C#N)N	organic		1.30%	4.80%	3.6923	High-Performance Green Light-Emitting Diodes Based on MAPbBr3 with π-Conjugated Ligand	https://doi.org/10.1021/acsami.0c02923	qutatum dots	2020
22	CsPbBr3	sodium citrate	C(C(=O)[O-])C(CC(=O)[O-])(C(=O)[O-])O.[Na+].[Na+].[Na+]	inorganic	6.000	5.60%	13.20%	2.3571	Perovskite light-emitting diodes with low roll-off efficiency via interfacial ionic immobilization	https://doi.org/10.1016/j.cej.2021.132347	3D	2021
23	CsPbBr3	4-bromobenzoic acid	C1=CC(=CC=C1C(=O)O)Br	inorganic	0.402	4.80%	7.60%	1.5833	High-performance all-inorganic perovskite light-emitting diodes enabled by a self-assembled molecule additive via defect passivation and strain	https://doi.org/10.1016/j.jallcom.2023.172459	3D	2023
23	CsPbBr3	4-bromobenzoic acid	C1=CC(=CC=C1C(=O)O)Br	inorganic	2.010	4.80%	9.20%	1.9167	High-performance all-inorganic perovskite light-emitting diodes enabled by a self-assembled molecule additive via defect passivation and strain	https://doi.org/10.1016/j.jallcom.2023.172459	3D	2023
23	CsPbBr3	4-bromobenzoic acid	C1=CC(=CC=C1C(=O)O)Br	inorganic	1.206	4.80%	11.40%	2.3750	High-performance all-inorganic perovskite light-emitting diodes enabled by a self-assembled molecule additive via defect passivation and strain	https://doi.org/10.1016/j.jallcom.2023.172459	3D	2023
24	(S-MBA)2Csn–1PbnBr3n+1	(l)-tryptophan bromide	C1=CC=C2C(=C1)C(=CN2)C[C@@H](C(=O)O)[NH3+].[Br-]	inorganic	20.000	7.88%	14.32%	1.8173	Rearranging the Phase Distribution of Quasi-2D Perovskite for Efficient and Narrow Emission Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acs.jpclett.2c01059	quasi-2D	2022
25	PEA:CsPbBr3	1,4,8,11-tetraazacyclotetradecane	C1CNCCNCCCNCCNC1	inorganic	1.000	2.80%	9.63%	3.4393	Novel Lewis Base Cyclam Self-Passivation of Perovskites without an Anti-Solvent Process for Efficient Light-Emitting Diodes	https://doi.org/10.1021/acsami.0c02768	quasi-2D	2022
25	PEA:CsPbBr3	1,4,8,11-tetraazacyclotetradecane	C1CNCCNCCCNCCNC1	inorganic	3.000	2.80%	13.14%	4.6929	Novel Lewis Base Cyclam Self-Passivation of Perovskites without an Anti-Solvent Process for Efficient Light-Emitting Diodes	https://doi.org/10.1021/acsami.0c02768	quasi-2D	2022
25	PEA:CsPbBr3	1,4,8,11-tetraazacyclotetradecane	C1CNCCNCCCNCCNC1	inorganic	2.000	2.80%	16.24%	5.8000	Novel Lewis Base Cyclam Self-Passivation of Perovskites without an Anti-Solvent Process for Efficient Light-Emitting Diodes	https://doi.org/10.1021/acsami.0c02768	quasi-2D	2022
26	FA0.7MA0.1GA0.2)0.87Cs0.13PbB	benzylphosphonic acid	C1=CC=C(C=C1)CP(=O)(O)O	organic	17.969	6.10%	29.20%	4.7869	Ultra-bright, efficient and stable perovskite light-emitting diodes	://www-nature-com-443.webvpn.jnu.edu.cn/articles/s41586-022-05	3D	2022
27	PEA:CsPbBr3	formamidine sulfinic acid	C(=N)(N)S(=O)O	inorganic	0.649	15.90%	16.40%	1.0314	Multidentate Molecule Anchoring Halide Perovskite Surface and Regulating Crystallization Kinetics toward Efficient Light-Emitting Diodes	https://doi.org/10.1002/smll.202205336	quasi-2D	2022
27	PEA:CsPbBr3	formamidine sulfinic acid	C(=N)(N)S(=O)O	inorganic	0.108	15.90%	19.40%	1.2201	Multidentate Molecule Anchoring Halide Perovskite Surface and Regulating Crystallization Kinetics toward Efficient Light-Emitting Diodes	https://doi.org/10.1002/smll.202205336	quasi-2D	2022
27	PEA:CsPbBr3	formamidine sulfinic acid	C(=N)(N)S(=O)O	inorganic	0.216	15.90%	26.50%	1.6667	Multidentate Molecule Anchoring Halide Perovskite Surface and Regulating Crystallization Kinetics toward Efficient Light-Emitting Diodes	https://doi.org/10.1002/smll.202205336	quasi-2D	2022
28	(PEA)2FA4Pb5Br16	triphenylphosphine oxide	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC=C3	organic		15.90%	18.30%	1.1509	Phosphonate/Phosphine Oxide Dyad Additive for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/ange.202117374	quasi-2D	2022
28	(PEA)2FA4Pb5Br16	bis(4-chlorophenyl)(phenyl)phosphine	C1=CC=C(C=C1)P(=O)(C2=CC=C(C=C2)Cl)C3=CC=C(C=C3)Cl	organic		15.90%	19.10%	1.2013	Phosphonate/Phosphine Oxide Dyad Additive for Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/ange.202117374	quasi-2D	2022
29	PEA:FAPbBr3	1-Butyl-3-methylimidazolium bromide	CCCCN1C=C[N+](=C1)C.[Br-]	organic	0.876	8.20%	8.70%	1.0610	Targeted Distribution of Passivator for Polycrystalline Perovskite Light-Emitting Diodes with High Efficienc	https://pubs.acs.org/doi/10.1021/acsenergylett.1c01753	quasi-2D	2021
29	PEA:FAPbBr3	1-Butyl-3-methylimidazolium tetrafluoroborate(BMIMBF4)	[B-](F)(F)(F)F.CCCCN1C=C[N+](=C1)C	organic	0.452	8.20%	13.20%	1.6098	Targeted Distribution of Passivator for Polycrystalline Perovskite Light-Emitting Diodes with High Efficienc	https://pubs.acs.org/doi/10.1021/acsenergylett.1c01753	quasi-2D	2021
29	PEA:FAPbBr3	1-Butyl-3-methylimidazolium tetrafluoroborate(BMIMBF4)	[B-](F)(F)(F)F.CCCCN1C=C[N+](=C1)C	organic	1.808	8.20%	16.50%	2.0122	Targeted Distribution of Passivator for Polycrystalline Perovskite Light-Emitting Diodes with High Efficienc	https://pubs.acs.org/doi/10.1021/acsenergylett.1c01753	quasi-2D	2021
29	PEA:FAPbBr3	Formamidinium tetrafluoroborate	[B-](F)(F)(F)F.C(=[NH2+])N	organic	0.527	8.20%	18.90%	2.3049	Targeted Distribution of Passivator for Polycrystalline Perovskite Light-Emitting Diodes with High Efficienc	https://pubs.acs.org/doi/10.1021/acsenergylett.1c01753	quasi-2D	2021
29	PEA:FAPbBr3	1-Butyl-3-methylimidazolium tetrafluoroborate(BMIMBF4)	[B-](F)(F)(F)F.CCCCN1C=C[N+](=C1)C	organic	0.904	8.20%	22.90%	2.7927	Targeted Distribution of Passivator for Polycrystalline Perovskite Light-Emitting Diodes with High Efficienc	https://pubs.acs.org/doi/10.1021/acsenergylett.1c01753	quasi-2D	2021
30	FAPbBr3	1,3,5-tris (bromomethyl) benzene	C1=C(C=C(C=C1CBr)CBr)CBr	organic	0.091	16.00%	20.10%	1.2563	A Multi-functional Molecular Modifier Enabling Efficient Large-Area Perovskite Light-Emitting Diodes	https://www.cell.com/joule/fulltext/S2542-4351(20)30286-5#mmc1	3D	2020
31	CsPbBr3	2-Hydroxymethyl-12-crown-4	C1COCCOC(COCCO1)CO	inorganic	5.000	0.32%	1.18%	3.6875	Synergistic morphology control and non-radiative defect passivation using a crown ether for efficient perovskite light-emitting devices	https://doi.org/10.1039/D0TC02062A	film	2020
32	CsPbBr3	2,4,6-Tris[3-(diphenylphosphinyl)phenyl]-1,3,5-	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC(=C3)C4=NC(=NC(=N4)C5=CC(=CC=C5)P(=O)(C6=CC=CC=C6)C7	inorganic		13.00%	18.80%	1.4462	Interfacial Molecule Control Enables Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/adfm.202307818	3D	2023
33	PEA:CsPbBr3	l-norvaline	CCC[C@@H](C(=O)O)N	inorganic	8.000	4.09%	8.93%	2.1834	Suppressing Formation of Buried Defects during Annealing Enables Bright Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acsami.4c08637	quasi-2D	2024
33	PEA:CsPbBr3	l-norvaline	CCC[C@@H](C(=O)O)N	inorganic	2.000	4.09%	10.85%	2.6528	Suppressing Formation of Buried Defects during Annealing Enables Bright Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acsami.4c08637	quasi-2D	2024
33	PEA:CsPbBr3	l-norvaline	CCC[C@@H](C(=O)O)N	inorganic	5.000	4.09%	13.04%	3.1883	Suppressing Formation of Buried Defects during Annealing Enables Bright Perovskite Light-Emitting Diodes	https://doi.org/10.1021/acsami.4c08637	quasi-2D	2024
34	CsPbBr3	betaine	C[N+](C)(C)CC(=O)[O-]	inorganic	5.000	3.48%	11.11%	3.1925	Interfacial engineering for highly efficient quasi-two dimensional organic–inorganic hybrid perovskite light-emitting diodes	https://doi.org/10.1039/C8TC06490C	3D	2019
35	PEA:CsPbBr3	ibuprofen	CC(C)CC1=CC=C(C=C1)C(C)C(=O)O	inorganic	4.000	4.26%	8.90%	2.0892	Passivation in Quasi-2D Perovskite Light-Emitting Diodes by an Ibuprofen	https://pubs.acs.org/doi/10.1021/acsami.3c10337	quasi-2D	2023
35	PEA:CsPbBr3	ibuprofen	CC(C)CC1=CC=C(C=C1)C(C)C(=O)O	inorganic	1.000	4.26%	11.04%	2.5915	Defect Passivation in Quasi-2D Perovskite Light-Emitting Diodes by an Ibuprofen Additive	https://pubs.acs.org/doi/10.1021/acsami.3c10337	quasi-2D	2023
35	PEA:CsPbBr3	ibuprofen	CC(C)CC1=CC=C(C=C1)C(C)C(=O)O	inorganic	2.000	4.26%	14.70%	3.4507	Defect Passivation in Quasi-2D Perovskite Light-Emitting Diodes by an Ibuprofen Additive	https://pubs.acs.org/doi/10.1021/acsami.3c10337	quasi-2D	2023
36	CsPbBr3	thiocyanate	C(#N)[S-]	inorganic	8.712	12.00%	17.00%	1.4167	Pseudohalogen Resurfaced CsPbBr3 Nanocrystals for Bright, Efficient, and Stable Green-Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acs.nanolett.3c00385	3D	2023
37	Cs0.5MA0.4FA0.1PbBr3	triphenylphosphine oxide	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC=C3	inorganic	4.000	3.35%	10.28%	3.0687	Conductive Phosphine Oxide Passivator Enables Efficient Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acs.nanolett.2c00276	3D	2022
37	Cs0.5MA0.4FA0.1PbBr3	2,7-bis(diphenylphosphoryl)-9,9'-spirobifluorene	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC4=C(C=C3)C5=C(C46C7=CC=CC=C7C8=CC=CC=C68)C=C(C=C5)P(=	inorganic	4.000	3.35%	22.30%	6.6567	Conductive Phosphine Oxide Passivator Enables Efficient Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acs.nanolett.2c00276	3D	2022
38	CsPbBr3	2-phenylethanamine bromide	C1=CC=C(C=C1)CCN.Br	inorganic	1.000	1.27%	2.36%	1.8583	Improved Performance for Thermally Evaporated Perovskite Light-Emitting Devices via Defect Passivation and Carrier Regulation	https://pubs.acs.org/doi/10.1021/acsami.0c01173	3D	2020
38	CsPbBr3	2-phenylethanamine bromide	C1=CC=C(C=C1)CCN.Br	inorganic	2.500	1.27%	2.73%	2.1496	Improved Performance for Thermally Evaporated Perovskite Light-Emitting Devices via Defect Passivation and Carrier Regulation	https://pubs.acs.org/doi/10.1021/acsami.0c01173	3D	2020
38	CsPbBr3	2-phenylethanamine bromide	C1=CC=C(C=C1)CCN.Br	inorganic	2.000	1.27%	4.10%	3.2283	Improved Performance for Thermally Evaporated Perovskite Light-Emitting Devices via Defect Passivation and Carrier Regulation	https://pubs.acs.org/doi/10.1021/acsami.0c01173	3D	2020
39	MAPbBr3	benzyltrimethylammonium chloride (BTACl)	C[N+](C)(C)CC1=CC=CC=C1.[Cl-]	organic	12.000	0.19%	0.10%	0.5263	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	benzyltrimethylammonium chloride (BTACl)	C[N+](C)(C)CC1=CC=CC=C1.[Cl-]	organic	8.000	0.19%	0.15%	0.7895	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	phenyltrimethylammonium bromide (PTABr)	C[N+](C)(C)C1=CC=CC=C1.[Br-]	organic	6.000	0.19%	0.22%	1.1579	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	benzyltrimethylammonium bromide (BTABr)	C[N+](C)(C)CC1=CC=CC=C1.[Br-]	organic	12.000	0.19%	0.29%	1.5263	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	benzyltrimethylammonium chloride (BTACl)	C[N+](C)(C)CC1=CC=CC=C1.[Cl-]	organic	10.000	0.19%	0.30%	1.5789	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	phenyltrimethylammonium bromide (PTABr)	C[N+](C)(C)C1=CC=CC=C1.[Br-]	organic	10.000	0.19%	0.30%	1.5789	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	benzyltrimethylammonium bromide (BTABr)	C[N+](C)(C)CC1=CC=CC=C1.[Br-]	organic	8.000	0.19%	0.44%	2.3158	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	phenyltrimethylammonium bromide (PTABr)	C[N+](C)(C)C1=CC=CC=C1.[Br-]	organic	8.000	0.19%	0.52%	2.7368	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
39	MAPbBr3	benzyltrimethylammonium bromide (BTABr)	C[N+](C)(C)CC1=CC=CC=C1.[Br-]	organic	10.000	0.19%	1.03%	5.4211	Bright perovskite light-emitting diodes with improved film morphology and reduced trap density via surface passivation using quaternary ammonium	https://doi.org/10.1016/j.orgel.2019.01.030	3D	2019
40	CsPbBr3	betaine	C[N+](C)(C)CC(=O)[O-]	inorganic	20.000	3.10%	10.80%	3.4839	Stabilizing dynamic surface of highly luminescent perovskite quantum dots for light-emitting diodes	https://doi.org/10.1016/j.cej.2022.139909	qutatum dots	2022
41	PEA2Csn–1PbnBr3n+1	betaine citrate	C[N+](C)(C)CC(=O)O.C(C(=O)O)C(CC(=O)O)(C(=O)[O-])O	inorganic	3.000	14.70%	23.20%	1.5782	Universal Molecular Control Strategy for Scalable Fabrication of Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acs.nanolett.2c04459	3D	2023
42	PEA:CsPbBr3	[2-(3,6-dimethoxy-9H-carbazol-9-yl)ethyl]phosphonic acid	COC1=CC2=C(C=C1)N(C3=C2C=C(C=C3)OC)CCP(=O)(O)O	inorganic	1.000	2.31%	3.40%	1.4719	Fabrication of Highly Luminescent Quasi Two-Dimensional CsPbBr3 Perovskite Films in High Humidity Air for Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acsami.3c07140	quasi-2D	2023
42	PEA:CsPbBr3	[2-(9H-Carbazol-9-yl)ethyl]phosphonic acid	C1=CC=C2C(=C1)C3=CC=CC=C3N2CCP(=O)(O)O	inorganic	0.300	2.31%	4.26%	1.8442	Fabrication of Highly Luminescent Quasi Two-Dimensional CsPbBr3 Perovskite Films in High Humidity Air for Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acsami.3c07140	quasi-2D	2023
43	BA2Csn-1PbnBr3n+1	3, 6-Dibromocarbazole	C1=CC2=C(C=C1Br)C3=C(N2)C=CC(=C3)Br	inorganic	3.000	13.87%	14.29%	1.0303	Effective Small Organic Molecule as a Defect Passivator for Highly Efficient Quasi-2D Perovskite Light-Emitting Diodes	https://doi.org/10.1002/smll.202308847	quasi-2D	2023

43	BA2Csn-1PbnBr3n+1	2, 8-Dibromodibenzothiophene	C1=CC2=C(C=C1Br)C3=C(S2)C=CC(=C3)Br	inorganic	3.000	13.87%	16.20%	1.1680	Effective Small Organic Molecule as a Defect Passivator for Highly Efficient Quasi-2D Perovskite Light-Emitting Diodes	https://doi.org/10.1002/smll.202308847	quasi-2D	2023
43	BA2Csn-1PbnBr3n+1	2, 8-dibromodibenzofuran	C1=CC2=C(C=C1Br)C3=C(O2)C=CC(=C3)Br	inorganic	3.000	13.87%	19.90%	1.4348	Effective Small Organic Molecule as a Defect Passivator for Highly Efficient Quasi-2D Perovskite Light-Emitting Diodes	https://doi.org/10.1002/smll.202308847	quasi-2D	2023
44	PEA2(FAPbBr3)2PbBr4	2-(methylsulfonyl)-4-(trifluoromethyl)benzoic acid	CS(=O)(=O)C1=C(C=CC(=C1)C(F)(F)F)C(=O)O	organic	8.046	16.80%	25.90%	1.5417	Multiple Phase Regulation Enables Efficient and Bright Quasi-2D Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acs.nanolett.3c03440	quasi-2D	2023
45	CsPbBr3	4-amino-N-methylphthalimide	CN1C(=O)C2=C(C1=O)C=C(C=C2)N	inorganic	0.881	1.08%	1.91%	1.7685	Highly effective surface defect passivation of perovskite quantum dots for excellent optoelectronic properties	https://doi.org/10.1016/j.jmrt.2022.04.080	quantum dots	2022
46	PEA2(FAPbBr3)2PbBr4	Potassium tetrafluoroborate	[B-](F)(F)(F)F.[K+]	organic	0.755	6.25%	10.46%	1.6736	Modulating phase distribution and passivating surface defects of quasi-2D perovskites via potassium tetrafluoroborate for light-emitting diodes	https://doi.org/10.1016/j.cej.2022.138021	quasi-2D	2022
46	PEA2(FAPbBr3)2PbBr4	Potassium tetrafluoroborate	[B-](F)(F)(F)F.[K+]	organic	2.266	6.25%	13.92%	2.2272	Modulating phase distribution and passivating surface defects of quasi-2D perovskites via potassium tetrafluoroborate for light-emitting diodes	https://doi.org/10.1016/j.cej.2022.138021	quasi-2D	2022
47	FAPbBr3	1-(1-naphthyl)ethylamine bromide	C[C@H](C1=CC=CC2=CC=CC=C21)N.Br	organic		3.30%	8.60%	2.6061	Modulation of ligand conjugation for efficient FAPbBr3 based green light-emitting diodes	https://doi.org/10.1039/C9QM00768G	3D	2020
48	CsPbBr3	Butyl(2-ethylhexyl)dimethylammonium bromide	CCCCC(CC)C[N+](C)(C)CCCC.[Br-]	inorganic		6.31%	23.45%	3.7163	In Situ Ligand Compensation of Perovskite Quantum Dots for Efficient Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acsenergylett.3c01686	quantum dots	2023
49	CsPbBr3	hexanoic acid sodium salt	CCCCCC(=O)[O-].[Na+]	inorganic	2.763	2.80%	3.30%	1.1786	Hard and soft Lewis-base behavior for efficient and stable CsPbBr3 perovskite light-emitting diodes	https://doi.org/10.1515/nanoph-2021-0003	3D	2021
49	$CsPbBr_3$	benzoic acid sodium salt	C1=CC=C(C=C1)C(=O)[O-].[Na+]	inorganic	2.882	2.08%	11.42%	5.4904	Hard and soft Lewis-base behavior for efficient and stable CsPbBr3 perovskite light-emitting diodes	https://doi.org/10.1515/nanoph-2021-0003	3D	2021
49	$CsPbBr_3$	4-(trifluoromethyl) benzoate acid sodium salt	C1=CC(=C(C=C1C(F)(F)F)Cl)OC2=CC(=C(C=C2)[N+](=O)[O-])C(=O)[O-].[Na+]	inorganic	4.242	2.08%	16.75%	8.0529	Hard and soft Lewis-base behavior for efficient and stable CsPbBr3 perovskite light-emitting diodes	https://doi.org/10.1515/nanoph-2021-0003	3D	2021
50	PEA:FAPbBr3	methyldiphenylphosphine oxide	CP(=O)(C1=CC=CC=C1)C2=CC=CC=C2	organic	0.995	19.00%	21.57%	1.1353	Insight into Diphenyl Phosphine Oxygen-Based Molecular Additives as Defect Passivators toward Efficient Quasi-2D Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acsami.2c19646	quasi-2D	2023
50	PEA:FAPbBr3	diphenylphosphine oxide	C1=CC=C(C=C1)[P+](=O)C2=CC=CC=C2	organic	0.925	19.00%	21.98%	1.1568	Insight into Diphenyl Phosphine Oxygen-Based Molecular Additives as Defect Passivators toward Efficient Quasi-2D Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acsami.2c19646	quasi-2D	2023
50	PEA:FAPbBr3	diphenylphosphinic acid	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)O	organic	1.004	19.00%	22.44%	1.1811	Insight into Diphenyl Phosphine Oxygen-Based Molecular Additives as Defect Passivators toward Efficient Quasi-2D Perovskite Light-Emitting Diodes	https://pubs.acs.org/doi/10.1021/acsami.2c19646	quasi-2D	2023
51	(FAMA)0.5Cs0.5PbI3	triphenylphosphine oxide	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC=C3	organic	12.000	19.10%	21.01%	1.1000	Efficient Perovskite Light-Emitting Diodes by Buried Interface Modification with Triphenylphosphine Oxide	https://pubs.acs.org/doi/10.1021/acsami.2c19123	3D	2023
52	FAPbBr3	2-naphthalenesulfonic acid	C1=CC=C2C=C(C=CC2=C1)S(=O)(=O)O	organic	1.000	13.30%	19.20%	1.4436	High-Brightness Perovskite Light-Emitting Diodes Based on FAPbBr3 Nanocrystals with Rationally Designed Aromatic Ligands	https://pubs.acs.org/doi/10.1021/acsenergylett.1c00812	3D	2021
53	CH3NH3PbBr3	thiophenol	C1=CC=C(C=C1)S	organic	0.331	2.20%	2.63%	1.1955	Case Studies on Structure–Property Relations in Perovskite Light-Emitting Diodes via Interfacial Engineering with Self-Assembled Monolayers	https://pubs.acs.org/doi/10.1021/acsami.1c03797	film	2021
53	CH3NH3PbBr3	cysteamine	C(CS)N	organic	0.231	2.20%	4.21%	1.9136	Case Studies on Structure–Property Relations in Perovskite Light-Emitting Diodes via Interfacial Engineering with Self-Assembled Monolayers	https://pubs.acs.org/doi/10.1021/acsami.1c03797	film	2021
53	CH3NH3PbBr3	4-aminothiophenol	C1=CC(=CC=C1N)S	organic	0.376	2.20%	4.75%	2.1591	Case Studies on Structure–Property Relations in Perovskite Light-Emitting Diodes via Interfacial Engineering with Self-Assembled Monolayers	https://pubs.acs.org/doi/10.1021/acsami.1c03797	film	2021
53	CH3NH3PbBr3	4-mercaptopyridine	C1=CNC=CC1=S	organic	0.334	2.20%	5.74%	2.6091	Case Studies on Structure–Property Relations in Perovskite Light-Emitting Diodes via Interfacial Engineering with Self-Assembled Monolayers	https://pubs.acs.org/doi/10.1021/acsami.1c03797	film	2021
54	CsPbBr3	3-(decyldimethylammonio)propanesulfonate	CCCCCCCCCC[N+](C)(C)CCCS(=O)(=O)[O-]	inorganic	30.750	5.10%	12.17%	2.3863	Efficient CsPbBr3 Perovskite Light-Emitting Diodes via Novel Multi-Step Ligand Exchange Strategy Based on Zwitterionic Molecules	https://pubs.acs.org/doi/10.1021/acsami.3c17324	quantum dots	2024
54	CsPbBr3	dodecyl dimethylamine bromide	CCCCCCCCCCCCN(C)C.Br	inorganic	8.829	1.79%	5.11%	2.8547	Efficient CsPbBr3 Perovskite Light-Emitting Diodes via Novel Multi-Step Ligand Exchange Strategy Based on Zwitterionic Molecules	https://pubs.acs.org/doi/10.1021/acsami.3c17324	quantum dots	2024
55	PEA 2 (FAPbBr 3) 4 PbBr 4	potassium bromide	[K+].[Br-]	organic	11.900	13.60%	20.83%	1.5316	Enhancing the Performance of Perovskite Light-Emitting Diodes via Synergistic Effect of Defect Passivation and Dielectric Screening	https://link.springer.com/article/10.1007/s40820-024-01405-5	quasi-2D	2024
56	PEA:CsPbBr3	1-butyl-3-methylimidazolium trifluoromethanesulfonate	CCCCN1C=C[N+](=C1)C.C(F)(F)(F)S(=O)(=O)[O-]	inorganic	1.000	7.60%	12.70%	1.6711	A Multifunctional Ionic Liquid Additive Enabling Stable and Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/smll.202200498	quasi-2D	2022
56	PEA:CsPbBr3	1-butyl-3-methylimidazolium trifluoromethanesulfonate	CCCCN1C=C[N+](=C1)C.C(F)(F)(F)S(=O)(=O)[O-]	inorganic	3.000	7.60%	14.50%	1.9079	A Multifunctional Ionic Liquid Additive Enabling Stable and Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/smll.202200498	quasi-2D	2022
56	PEA:CsPbBr3	1-butyl-3-methylimidazolium trifluoromethanesulfonate	CCCCN1C=C[N+](=C1)C.C(F)(F)(F)S(=O)(=O)[O-]	inorganic	2.000	7.60%	17.60%	2.3158	A Multifunctional Ionic Liquid Additive Enabling Stable and Efficient Perovskite Light-Emitting Diodes	https://doi.org/10.1002/smll.202200498	quasi-2D	2022
57	CsPbBr3	(2-(9H-Carbazol-9-yl)ethyl)phosphonic acid	C1=CC=C2C(=C1)C3=CC=CC=C3N2CCP(=O)(O)O	inorganic	3.000	7.93%	20.87%	2.6318	Efficient All-Inorganic Perovskite Light-Emitting Diodes Enabled by Simultaneous Growth Regulation and Defect Passivation	https://doi.org/10.1109/TED.2024.3418724	3D	2024
58	PEA: CsPbBr3	potassium thiocyanate	C(#N)[S-].[K+]	inorganic	2.915	9.10%	16.30%	1.7912	Low-dimensional phase suppression and defect passivation of quasi-2D perovskites for efficient electroluminescence and low-threshold amplified spontaneous emission	https://doi.org/10.1039/D1NR06549A	quasi-2D	2022
58	PEA: CsPbBr3	butylammonium bromide	CCCCN.Br	inorganic	9.243	1.90%	9.10%	4.7895	Low-dimensional phase suppression and defect passivation of quasi-2D perovskites for efficient electroluminescence and low-threshold amplified	https://doi.org/10.1039/D1NR06549A	quasi-2D	2022
59	PEA: CsPbBr3	pentafluorophenyl diphenylphosphinate	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)OC3=C(C(=C(C(=C3F)F)F)F)F	inorganic	5.000	14.92%	15.98%	1.0710	Efficient Quasi-Two-Dimensional Perovskite Light-Emitting Diodes Achieved through the Passivation of Multi-Fluorine Phosphate Molecules	https://doi.org/10.3390/mi15060799	quasi-2D	2024
59	PEA: CsPbBr3	pentafluorophenyl diphenylphosphinate	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)OC3=C(C(=C(C(=C3F)F)F)F)F	inorganic	10.000	14.92%	17.76%	1.1903	Efficient Quasi-Two-Dimensional Perovskite Light-Emitting Diodes Achieved through the Passivation of Multi-Fluorine Phosphate Molecules	https://doi.org/10.3390/mi15060799	quasi-2D	2024
59	PEA: CsPbBr3	pentafluorophenyl diphenylphosphinate	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)OC3=C(C(=C(C(=C3F)F)F)F)F	inorganic	20.000	14.92%	18.53%	1.2420	Efficient Quasi-Two-Dimensional Perovskite Light-Emitting Diodes Achieved through the Passivation of Multi-Fluorine Phosphate Molecules	https://doi.org/10.3390/mi15060799	quasi-2D	2024
59	PEA: CsPbBr3	pentafluorophenyl diphenylphosphinate	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)OC3=C(C(=C(C(=C3F)F)F)F)F	inorganic	15.000	14.92%	21.06%	1.4115	Efficient Quasi-Two-Dimensional Perovskite Light-Emitting Diodes Achieved through the Passivation of Multi-Fluorine Phosphate Molecules	https://doi.org/10.3390/mi15060799	quasi-2D	2024
60	CsPbBr3	didodecyldimethylammonium bromide	CCCCCCCCCCCC[N+](C)(C)CCCCCCCCCCCC.[Br-]	inorganic	1.600	1.78%	3.91%	2.1966	Heterogeneous post-passivation of inorganic cesium lead halide perovskite quantum dots for efficient electroluminescent devices	https://doi.org/10.1039/D0TC05856D	quantum dots	2021
60	CsPbBr3	formamidinium bromide	C(=[NH2+])N.[Br-]	inorganic	3.200	1.78%	7.94%	4.4607	Heterogeneous post-passivation of inorganic cesium lead halide perovskite quantum dots for efficient electroluminescent devices	https://doi.org/10.1039/D0TC05856D	quantum dots	2021
61	MAPbBr3	2,2',2''-(1,3,5-benzinetriyl)-tris(1-phenyl-1-H-benzimidazole	C1=CC=C(C=C1)N2C3=CC=CC=C3N=C2C4=CC(=CC(=C4)C5=NC6=CC=CC=C6N5C7=CC=CC=C7)C8=NC9=CC=CC=C9N8C1=CC=CC=C1	organic		8.64%	11.70%	1.3542	Efficient Perovskite Light-Emitting Diodes Using Polycrystalline Core–Shell-Mimicked Nanograins	https://doi.org/10.1002/adfm.201902017	3D	2019
62	CsPbBr3	1,3,5-tris(1-phenyl-1H-benzimidazol-2-yl) benzene	C1=CC=C(C=C1)N2C3=CC=CC=C3N=C2C4=CC(=CC(=C4)C5=NC6=CC=CC=C6N5C7=CC=CC=C7)C8=NC9=CC=CC=C9N8C1=CC=CC=C1	inorganic	3.000	13.50%	17.50%	1.2963	Efficient Perovskite Light-Emitting Diodes with Chemically Bonded Contact and Regulated Charge Behavior	https://doi.org/10.1021/acs.nanolett.3c02335	3D	2023
62	CsPbBr3	2,4,6-tris[3-(diphenylphosphinyl)phenyl]-1,3,5-triazine	C1=CC=C(C=C1)P(=O)(C2=CC=CC=C2)C3=CC=CC(=C3)C4=NC(=NC(=N4)C5=CC(=CC=C5)P(=O)(C6=CC=CC=C6)C7=CC=CC=C7)C8=CC(=CC=C8)P(=O)(C9=CC=CC=C9)C1=C	inorganic	3.000	13.50%	22.06%	1.6341	Efficient Perovskite Light-Emitting Diodes with Chemically Bonded Contact and Regulated Charge Behavior	https://doi.org/10.1021/acs.nanolett.3c02335	3D	2023

Constructed Prediction dataset

Num	CID	IUPACName	MolecularFormula	Isomeric SMILES	A_site	Conc(mg/ml)	H_Acceptors	H_Donors	Rot_bonds	Mol_Wt	TPSA	Avglpc	Hydrogen	Oxide	Notrigen	Halide
1	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	0	1	1	1	1	127.574	26.02	2.1120661	6	0	1	1
2	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	0	1	3	1	2	138.126	69.16	2.1311082	6	2	2	0
3	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	0	1	1	1	1	111.119	26.02	2.1120661	6	0	1	1
4	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	0	1	4	1	4	168.152	78.39	2.2222351	8	3	2	0
5	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	0	1	3	1	3	152.153	69.16	2.1964662	8	2	2	0
6	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	0	1	3	1	3	171.221	60.16	2.2423094	9	2	1	0
7	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	0	1	4	1	6	196.206	78.39	2.4160557	12	3	2	0
8	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	0	1	3	1	2	178.235	38.49	2.4591717	14	1	2	0
9	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	0	1	3	1	2	172.571	69.16	2.1837138	5	2	2	1
10	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	0	1	3	1	2	225.191	60.16	2.2423094	6	2	1	3
11	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	0	1	1	1	1	470.817	26.02	2.1120661	4	0	1	3
12	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	0	1	3	1	4	166.18	69.16	2.2238177	10	2	2	0
13	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	0	1	2	1	7	144.214	37.3	2.4325145	16	2	0	0
14	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	0	1	3	2	3	90.078	57.53	1.9894655	6	3	0	0
15	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	0	1	3	2	2	137.138	63.32	2.2585839	7	2	1	0
16	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	0	1	5	4	4	170.12	97.99	2.3720847	6	5	0	0
17	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	0	1	5	2	2	167.12	87.49	2.3315544	5	4	1	0
18	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	0	1	4	3	1	156.097	103.02	2.2319352	4	4	2	0
19	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	0	1	3	2	1	189.17	70.16	2.4576751	7	3	1	0
20	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	0	1	3	1	5	179.219	50.19	2.4790777	13	2	1	0
21	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	0	1	2	0	2	137.138	44.01	2.1129569	7	2	1	0
22	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	0	1	3	2	1	139.11	70.16	2.2319352	5	3	1	0
23	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	0	1	2	1	1	122.127	55.98	2.137382	6	1	2	0
24	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	0	1	1	0	1	106.124	17.07	2.1120661	6	1	0	0
25	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	0	1	3	2	4	214.22	57.53	2.5966697	10	3	0	0
26	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	0	1	7	0	2	322.228	103.81	3.1278468	6	7	0	0
27	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	0	1	3	0	3	165.148	60.21	2.2477146	7	3	1	0
28	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	0	1	3	4	0	146.106	127.31	2.2290666	6	3	4	0
29	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	0	1	2	0	3	138.619	17.07	1.7991202	7	1	0	1
30	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	0	1	4	2	3	189.171	87.74	2.3757381	11	4	3	0
31	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	0	1	3	1	2	158.201	41.57	2.3260104	14	2	2	0
32	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	0	1	1	0	1	158.559	17.07	2.1120661	4	1	0	2
33	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	0	1	1	0	0	224.348	23.55	2.7142256	24	1	2	0
34	1176	urea	CH4N2O	C(=O)(N)N	0	1	1	2	0	60.056	69.11	1.6403361	4	1	2	0
35	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	0	1	1	0	3	134.178	17.07	2.2423094	10	1	0	0
36	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	0	1	1	0	4	148.205	17.07	2.3420428	12	1	0	0
37	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	0	1	3	1	2	139.11	63.37	2.1552786	5	3	1	0
38	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	0	1	3	0	4	105.093	52.37	1.7991202	7	3	1	0
39	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	0	1	5	0	3	121.048	78.67	1.7988538	3	5	1	0
40	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	0	1	3	0	9	175.228	52.37	2.4078886	17	3	1	0
41	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	0	1	3	0	7	147.174	52.37	2.2378826	13	3	1	0
42	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	0	1	6	0	9	275.197	87.9	2.5331818	14	6	1	0
43	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	0	1	2	0	1	123.111	43.14	2.1120661	5	2	1	0
44	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	0	1	4	1	3	119.076	80.44	2.0170171	5	4	1	0
45	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	0	1	5	1	3	184.107	106.51	2.214052	4	5	2	0
46	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	0	1	3	0	1	190.158	70.08	2.3885948	6	3	2	0
47	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	0	1	3	1	2	138.126	69.16	2.1400209	6	2	2	0
48	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	0	1	2	0	1	260.891	43.14	2.1120661	1	2	1	4
49	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	0	1	3	1	2	207.016	69.16	2.1400209	4	2	2	2
50	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	0	1	4	0	2	168.108	86.28	2.1400209	4	4	2	0
51	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	0	1	2	0	1	249.007	43.14	2.1120661	4	2	1	1
52	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	0	1	7	0	14	290.189	80.29	2.4562006	20	7	0	0
53	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	0	1	4	0	15	266.318	44.76	2.680459	27	4	0	0
54	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	0	1	4	1	5	126.048	55.76	1.7790463	7	4	0	0
55	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	0	1	6	3	7	170.057	104.06	2.2680478	7	6	0	0
56	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	0	1	4	0	9	182.156	44.76	2.1906621	15	4	0	0
57	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	0	1	4	1	19	322.426	55.76	2.9151042	35	4	0	0
58	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	0	1	4	1	7	154.102	55.76	2.114427	11	4	0	0
59	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	0	1	5	3	6	141.063	92.78	2.1606935	8	4	1	0
60	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	0	1	4	3	4	111.037	83.55	2.0205256	6	3	1	0
61	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	0	1	8	1	7	340.184	142.04	2.7103774	9	8	2	0
62	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	0	1	4	2	4	174.092	66.76	2.3859258	7	4	0	0
63	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	0	1	3	0	6	137.095	35.53	1.9512078	10	3	0	0
64	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	0	1	4	2	6	140.075	66.76	2.1466723	9	4	0	0
65	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	0	1	3	0	10	193.203	35.53	2.4183363	18	3	0	0
66	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	0	1	3	2	10	194.211	57.53	2.5804339	19	3	0	0
67	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	0	1	2	0	1	176.624	34.14	2.0946397	5	2	0	1
68	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	0	1	2	1	15	256.43	37.3	2.8959199	32	2	0	0
69	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	0	1	1	0	1	178.615	17.07	2.1120661	4	1	0	2
70	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	0	1	1	0	1	160.625	17.07	2.1120661	5	1	0	1
71	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	0	2	1	1	1	127.574	26.02	2.1120661	6	0	1	1
72	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	0	2	3	1	2	138.126	69.16	2.1311082	6	2	2	0
73	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	0	2	1	1	1	111.119	26.02	2.1120661	6	0	1	1
74	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	0	2	4	1	4	168.152	78.39	2.2222351	8	3	2	0
75	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	0	2	3	1	3	152.153	69.16	2.1964662	8	2	2	0
76	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	0	2	3	1	3	171.221	60.16	2.2423094	9	2	1	0
77	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	0	2	4	1	6	196.206	78.39	2.4160557	12	3	2	0
78	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	0	2	3	1	2	178.235	38.49	2.4591717	14	1	2	0
79	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	0	2	3	1	2	172.571	69.16	2.1837138	5	2	2	1
80	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	0	2	3	1	2	225.191	60.16	2.2423094	6	2	1	3
81	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	0	2	1	1	1	470.817	26.02	2.1120661	4	0	1	3
82	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	0	2	3	1	4	166.18	69.16	2.2238177	10	2	2	0
83	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	0	2	2	1	7	144.214	37.3	2.4325145	16	2	0	0
84	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	0	2	3	2	3	90.078	57.53	1.9894655	6	3	0	0
85	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	0	2	3	2	2	137.138	63.32	2.2585839	7	2	1	0
86	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	0	2	5	4	4	170.12	97.99	2.3720847	6	5	0	0
87	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	0	2	5	2	2	167.12	87.49	2.3315544	5	4	1	0
88	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	0	2	4	3	1	156.097	103.02	2.2319352	4	4	2	0
89	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	0	2	3	2	1	189.17	70.16	2.4576751	7	3	1	0
90	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	0	2	3	1	5	179.219	50.19	2.4790777	13	2	1	0
91	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	0	2	2	0	2	137.138	44.01	2.1129569	7	2	1	0
92	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	0	2	3	2	1	139.11	70.16	2.2319352	5	3	1	0
93	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	0	2	2	1	1	122.127	55.98	2.137382	6	1	2	0
94	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	0	2	1	0	1	106.124	17.07	2.1120661	6	1	0	0
95	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	0	2	3	2	4	214.22	57.53	2.5966697	10	3	0	0
96	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	0	2	7	0	2	322.228	103.81	3.1278468	6	7	0	0
97	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	0	2	3	0	3	165.148	60.21	2.2477146	7	3	1	0
98	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	0	2	3	4	0	146.106	127.31	2.2290666	6	3	4	0
99	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	0	2	2	0	3	138.619	17.07	1.7991202	7	1	0	1
100	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	0	2	4	2	3	189.171	87.74	2.3757381	11	4	3	0
101	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	0	2	3	1	2	158.201	41.57	2.3260104	14	2	2	0
102	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	0	2	1	0	1	158.559	17.07	2.1120661	4	1	0	2
103	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	0	2	1	0	0	224.348	23.55	2.7142256	24	1	2	0
104	1176	urea	CH4N2O	C(=O)(N)N	0	2	1	2	0	60.056	69.11	1.6403361	4	1	2	0
105	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	0	2	1	0	3	134.178	17.07	2.2423094	10	1	0	0
106	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	0	2	1	0	4	148.205	17.07	2.3420428	12	1	0	0
107	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	0	2	3	1	2	139.11	63.37	2.1552786	5	3	1	0
108	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	0	2	3	0	4	105.093	52.37	1.7991202	7	3	1	0
109	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	0	2	5	0	3	121.048	78.67	1.7988538	3	5	1	0
110	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	0	2	3	0	9	175.228	52.37	2.4078886	17	3	1	0
111	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	0	2	3	0	7	147.174	52.37	2.2378826	13	3	1	0
112	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	0	2	6	0	9	275.197	87.9	2.5331818	14	6	1	0
113	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	0	2	2	0	1	123.111	43.14	2.1120661	5	2	1	0
114	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	0	2	4	1	3	119.076	80.44	2.0170171	5	4	1	0
115	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	0	2	5	1	3	184.107	106.51	2.214052	4	5	2	0
116	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	0	2	3	0	1	190.158	70.08	2.3885948	6	3	2	0
117	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	0	2	3	1	2	138.126	69.16	2.1400209	6	2	2	0
118	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	0	2	2	0	1	260.891	43.14	2.1120661	1	2	1	4
119	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	0	2	3	1	2	207.016	69.16	2.1400209	4	2	2	2
120	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	0	2	4	0	2	168.108	86.28	2.1400209	4	4	2	0
121	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	0	2	2	0	1	249.007	43.14	2.1120661	4	2	1	1
122	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	0	2	7	0	14	290.189	80.29	2.4562006	20	7	0	0
123	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	0	2	4	0	15	266.318	44.76	2.680459	27	4	0	0
124	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	0	2	4	1	5	126.048	55.76	1.7790463	7	4	0	0
125	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	0	2	6	3	7	170.057	104.06	2.2680478	7	6	0	0
126	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	0	2	4	0	9	182.156	44.76	2.1906621	15	4	0	0
127	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	0	2	4	1	19	322.426	55.76	2.9151042	35	4	0	0
128	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	0	2	4	1	7	154.102	55.76	2.114427	11	4	0	0
129	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	0	2	5	3	6	141.063	92.78	2.1606935	8	4	1	0
130	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	0	2	4	3	4	111.037	83.55	2.0205256	6	3	1	0
131	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	0	2	8	1	7	340.184	142.04	2.7103774	9	8	2	0
132	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	0	2	4	2	4	174.092	66.76	2.3859258	7	4	0	0
133	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	0	2	3	0	6	137.095	35.53	1.9512078	10	3	0	0
134	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	0	2	4	2	6	140.075	66.76	2.1466723	9	4	0	0
135	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	0	2	3	0	10	193.203	35.53	2.4183363	18	3	0	0
136	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	0	2	3	2	10	194.211	57.53	2.5804339	19	3	0	0
137	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	0	2	2	0	1	176.624	34.14	2.0946397	5	2	0	1
138	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	0	2	2	1	15	256.43	37.3	2.8959199	32	2	0	0
139	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	0	2	1	0	1	178.615	17.07	2.1120661	4	1	0	2
140	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	0	2	1	0	1	160.625	17.07	2.1120661	5	1	0	1
141	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	0	4	1	1	1	127.574	26.02	2.1120661	6	0	1	1
142	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	0	4	3	1	2	138.126	69.16	2.1311082	6	2	2	0
143	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	0	4	1	1	1	111.119	26.02	2.1120661	6	0	1	1
144	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	0	4	4	1	4	168.152	78.39	2.2222351	8	3	2	0
145	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	0	4	3	1	3	152.153	69.16	2.1964662	8	2	2	0

146	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	0	4	3	1	3	171.221	60.16	2.2423094	9	2	1	0
147	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	0	4	4	1	6	196.206	78.39	2.4160557	12	3	2	0
148	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	0	4	3	1	2	178.235	38.49	2.4591717	14	1	2	0
149	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	0	4	3	1	2	172.571	69.16	2.1837138	5	2	2	1
150	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	0	4	3	1	2	225.191	60.16	2.2423094	6	2	1	3
151	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	0	4	1	1	1	470.817	26.02	2.1120661	4	0	1	3
152	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	0	4	3	1	4	166.18	69.16	2.2238177	10	2	2	0
153	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	0	4	2	1	7	144.214	37.3	2.4325145	16	2	0	0
154	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	0	4	3	2	3	90.078	57.53	1.9894655	6	3	0	0
155	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	0	4	3	2	2	137.138	63.32	2.2585839	7	2	1	0
156	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	0	4	5	4	4	170.12	97.99	2.3720847	6	5	0	0
157	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	0	4	5	2	2	167.12	87.49	2.3315544	5	4	1	0
158	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	0	4	4	3	1	156.097	103.02	2.2319352	4	4	2	0
159	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	0	4	3	2	1	189.17	70.16	2.4576751	7	3	1	0
160	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	0	4	3	1	5	179.219	50.19	2.4790777	13	2	1	0
161	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	0	4	2	0	2	137.138	44.01	2.1129569	7	2	1	0
162	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	0	4	3	2	1	139.11	70.16	2.2319352	5	3	1	0
163	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	0	4	2	1	1	122.127	55.98	2.137382	6	1	2	0
164	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	0	4	1	0	1	106.124	17.07	2.1120661	6	1	0	0
165	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	0	4	3	2	4	214.22	57.53	2.5966697	10	3	0	0
166	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	0	4	7	0	2	322.228	103.81	3.1278468	6	7	0	0
167	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	0	4	3	0	3	165.148	60.21	2.2477146	7	3	1	0
168	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	0	4	3	4	0	146.106	127.31	2.2290666	6	3	4	0
169	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	0	4	2	0	3	138.619	17.07	1.7991202	7	1	0	1
170	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	0	4	4	2	3	189.171	87.74	2.3757381	11	4	3	0
171	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	0	4	3	1	2	158.201	41.57	2.3260104	14	2	2	0
172	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	0	4	1	0	1	158.559	17.07	2.1120661	4	1	0	2
173	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	0	4	1	0	0	224.348	23.55	2.7142256	24	1	2	0
174	1176	urea	CH4N2O	C(=O)(N)N	0	4	1	2	0	60.056	69.11	1.6403361	4	1	2	0
175	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	0	4	1	0	3	134.178	17.07	2.2423094	10	1	0	0
176	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	0	4	1	0	4	148.205	17.07	2.3420428	12	1	0	0
177	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	0	4	3	1	2	139.11	63.37	2.1552786	5	3	1	0
178	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	0	4	3	0	4	105.093	52.37	1.7991202	7	3	1	0
179	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	0	4	5	0	3	121.048	78.67	1.7988538	3	5	1	0
180	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	0	4	3	0	9	175.228	52.37	2.4078886	17	3	1	0
181	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	0	4	3	0	7	147.174	52.37	2.2378826	13	3	1	0
182	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	0	4	6	0	9	275.197	87.9	2.5331818	14	6	1	0
183	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	0	4	2	0	1	123.111	43.14	2.1120661	5	2	1	0
184	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	0	4	4	1	3	119.076	80.44	2.0170171	5	4	1	0
185	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	0	4	5	1	3	184.107	106.51	2.214052	4	5	2	0
186	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	0	4	3	0	1	190.158	70.08	2.3885948	6	3	2	0
187	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	0	4	3	1	2	138.126	69.16	2.1400209	6	2	2	0
188	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	0	4	2	0	1	260.891	43.14	2.1120661	1	2	1	4
189	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	0	4	3	1	2	207.016	69.16	2.1400209	4	2	2	2
190	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	0	4	4	0	2	168.108	86.28	2.1400209	4	4	2	0
191	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	0	4	2	0	1	249.007	43.14	2.1120661	4	2	1	1
192	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	0	4	7	0	14	290.189	80.29	2.4562006	20	7	0	0
193	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	0	4	4	0	15	266.318	44.76	2.680459	27	4	0	0
194	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	0	4	4	1	5	126.048	55.76	1.7790463	7	4	0	0
195	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	0	4	6	3	7	170.057	104.06	2.2680478	7	6	0	0
196	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	0	4	4	0	9	182.156	44.76	2.1906621	15	4	0	0
197	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	0	4	4	1	19	322.426	55.76	2.9151042	35	4	0	0
198	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	0	4	4	1	7	154.102	55.76	2.114427	11	4	0	0
199	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	0	4	5	3	6	141.063	92.78	2.1606935	8	4	1	0
200	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	0	4	4	3	4	111.037	83.55	2.0205256	6	3	1	0
201	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	0	4	8	1	7	340.184	142.04	2.7103774	9	8	2	0
202	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	0	4	4	2	4	174.092	66.76	2.3859258	7	4	0	0
203	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	0	4	3	0	6	137.095	35.53	1.9512078	10	3	0	0
204	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	0	4	4	2	6	140.075	66.76	2.1466723	9	4	0	0
205	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	0	4	3	0	10	193.203	35.53	2.4183363	18	3	0	0
206	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	0	4	3	2	10	194.211	57.53	2.5804339	19	3	0	0
207	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	0	4	2	0	1	176.624	34.14	2.0946397	5	2	0	1
208	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	0	4	2	1	15	256.43	37.3	2.8959199	32	2	0	0
209	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	0	4	1	0	1	178.615	17.07	2.1120661	4	1	0	2
210	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	0	4	1	0	1	160.625	17.07	2.1120661	5	1	0	1
211	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	0	6	1	1	1	127.574	26.02	2.1120661	6	0	1	1
212	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	0	6	3	1	2	138.126	69.16	2.1311082	6	2	2	0
213	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	0	6	1	1	1	111.119	26.02	2.1120661	6	0	1	1
214	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	0	6	4	1	4	168.152	78.39	2.2222351	8	3	2	0
215	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	0	6	3	1	3	152.153	69.16	2.1964662	8	2	2	0
216	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	0	6	3	1	3	171.221	60.16	2.2423094	9	2	1	0
217	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	0	6	4	1	6	196.206	78.39	2.4160557	12	3	2	0
218	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	0	6	3	1	2	178.235	38.49	2.4591717	14	1	2	0
219	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	0	6	3	1	2	172.571	69.16	2.1837138	5	2	2	1
220	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	0	6	3	1	2	225.191	60.16	2.2423094	6	2	1	3
221	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	0	6	1	1	1	470.817	26.02	2.1120661	4	0	1	3
222	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	0	6	3	1	4	166.18	69.16	2.2238177	10	2	2	0
223	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	0	6	2	1	7	144.214	37.3	2.4325145	16	2	0	0
224	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	0	6	3	2	3	90.078	57.53	1.9894655	6	3	0	0
225	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	0	6	3	2	2	137.138	63.32	2.2585839	7	2	1	0
226	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	0	6	5	4	4	170.12	97.99	2.3720847	6	5	0	0
227	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	0	6	5	2	2	167.12	87.49	2.3315544	5	4	1	0
228	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	0	6	4	3	1	156.097	103.02	2.2319352	4	4	2	0
229	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	0	6	3	2	1	189.17	70.16	2.4576751	7	3	1	0
230	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	0	6	3	1	5	179.219	50.19	2.4790777	13	2	1	0
231	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	0	6	2	0	2	137.138	44.01	2.1129569	7	2	1	0
232	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	0	6	3	2	1	139.11	70.16	2.2319352	5	3	1	0
233	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	0	6	2	1	1	122.127	55.98	2.137382	6	1	2	0
234	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	0	6	1	0	1	106.124	17.07	2.1120661	6	1	0	0
235	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	0	6	3	2	4	214.22	57.53	2.5966697	10	3	0	0
236	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	0	6	7	0	2	322.228	103.81	3.1278468	6	7	0	0
237	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	0	6	3	0	3	165.148	60.21	2.2477146	7	3	1	0
238	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	0	6	3	4	0	146.106	127.31	2.2290666	6	3	4	0
239	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	0	6	2	0	3	138.619	17.07	1.7991202	7	1	0	1
240	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	0	6	4	2	3	189.171	87.74	2.3757381	11	4	3	0
241	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	0	6	3	1	2	158.201	41.57	2.3260104	14	2	2	0
242	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	0	6	1	0	1	158.559	17.07	2.1120661	4	1	0	2
243	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	0	6	1	0	0	224.348	23.55	2.7142256	24	1	2	0
244	1176	urea	CH4N2O	C(=O)(N)N	0	6	1	2	0	60.056	69.11	1.6403361	4	1	2	0
245	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	0	6	1	0	3	134.178	17.07	2.2423094	10	1	0	0
246	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	0	6	1	0	4	148.205	17.07	2.3420428	12	1	0	0
247	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	0	6	3	1	2	139.11	63.37	2.1552786	5	3	1	0
248	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	0	6	3	0	4	105.093	52.37	1.7991202	7	3	1	0
249	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	0	6	5	0	3	121.048	78.67	1.7988538	3	5	1	0
250	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	0	6	3	0	9	175.228	52.37	2.4078886	17	3	1	0
251	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	0	6	3	0	7	147.174	52.37	2.2378826	13	3	1	0
252	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	0	6	6	0	9	275.197	87.9	2.5331818	14	6	1	0
253	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	0	6	2	0	1	123.111	43.14	2.1120661	5	2	1	0
254	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	0	6	4	1	3	119.076	80.44	2.0170171	5	4	1	0
255	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	0	6	5	1	3	184.107	106.51	2.214052	4	5	2	0
256	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	0	6	3	0	1	190.158	70.08	2.3885948	6	3	2	0
257	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	0	6	3	1	2	138.126	69.16	2.1400209	6	2	2	0
258	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	0	6	2	0	1	260.891	43.14	2.1120661	1	2	1	4
259	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	0	6	3	1	2	207.016	69.16	2.1400209	4	2	2	2
260	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	0	6	4	0	2	168.108	86.28	2.1400209	4	4	2	0
261	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	0	6	2	0	1	249.007	43.14	2.1120661	4	2	1	1
262	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	0	6	7	0	14	290.189	80.29	2.4562006	20	7	0	0
263	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	0	6	4	0	15	266.318	44.76	2.680459	27	4	0	0
264	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	0	6	4	1	5	126.048	55.76	1.7790463	7	4	0	0
265	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	0	6	6	3	7	170.057	104.06	2.2680478	7	6	0	0
266	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	0	6	4	0	9	182.156	44.76	2.1906621	15	4	0	0
267	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	0	6	4	1	19	322.426	55.76	2.9151042	35	4	0	0
268	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	0	6	4	1	7	154.102	55.76	2.114427	11	4	0	0
269	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	0	6	5	3	6	141.063	92.78	2.1606935	8	4	1	0
270	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	0	6	4	3	4	111.037	83.55	2.0205256	6	3	1	0
271	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	0	6	8	1	7	340.184	142.04	2.7103774	9	8	2	0
272	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	0	6	4	2	4	174.092	66.76	2.3859258	7	4	0	0
273	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	0	6	3	0	6	137.095	35.53	1.9512078	10	3	0	0
274	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	0	6	4	2	6	140.075	66.76	2.1466723	9	4	0	0
275	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	0	6	3	0	10	193.203	35.53	2.4183363	18	3	0	0
276	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	0	6	3	2	10	194.211	57.53	2.5804339	19	3	0	0
277	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	0	6	2	0	1	176.624	34.14	2.0946397	5	2	0	1
278	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	0	6	2	1	15	256.43	37.3	2.8959199	32	2	0	0
279	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	0	6	1	0	1	178.615	17.07	2.1120661	4	1	0	2
280	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	0	6	1	0	1	160.625	17.07	2.1120661	5	1	0	1
281	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	0	8	1	1	1	127.574	26.02	2.1120661	6	0	1	1
282	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	0	8	3	1	2	138.126	69.16	2.1311082	6	2	2	0
283	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	0	8	1	1	1	111.119	26.02	2.1120661	6	0	1	1
284	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	0	8	4	1	4	168.152	78.39	2.2222351	8	3	2	0
285	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	0	8	3	1	3	152.153	69.16	2.1964662	8	2	2	0
286	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	0	8	3	1	3	171.221	60.16	2.2423094	9	2	1	0
287	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	0	8	4	1	6	196.206	78.39	2.4160557	12	3	2	0
288	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	0	8	3	1	2	178.235	38.49	2.4591717	14	1	2	0
289	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	0	8	3	1	2	172.571	69.16	2.1837138	5	2	2	1
290	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	0	8	3	1	2	225.191	60.16	2.2423094	6	2	1	3
291	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	0	8	1	1	1	470.817	26.02	2.1120661	4	0	1	3
292	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	0	8	3	1	4	166.18	69.16	2.2238177	10	2	2	0
293	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	0	8	2	1	7	144.214	37.3	2.4325145	16	2	0	0

294	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	0	8	3	2	3	90.078	57.53	1.9894655	6	3	0	0
295	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	0	8	3	2	2	137.138	63.32	2.2585839	7	2	1	0
296	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	0	8	5	4	4	170.12	97.99	2.3720847	6	5	0	0
297	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	0	8	5	2	2	167.12	87.49	2.3315544	5	4	1	0
298	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	0	8	4	3	1	156.097	103.02	2.2319352	4	4	2	0
299	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	0	8	3	2	1	189.17	70.16	2.4576751	7	3	1	0
300	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	0	8	3	1	5	179.219	50.19	2.4790777	13	2	1	0
301	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	0	8	2	0	2	137.138	44.01	2.1129569	7	2	1	0
302	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	0	8	3	2	1	139.11	70.16	2.2319352	5	3	1	0
303	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	0	8	2	1	1	122.127	55.98	2.137382	6	1	2	0
304	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	0	8	1	0	1	106.124	17.07	2.1120661	6	1	0	0
305	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	0	8	3	2	4	214.22	57.53	2.5966697	10	3	0	0
306	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	0	8	7	0	2	322.228	103.81	3.1278468	6	7	0	0
307	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	0	8	3	0	3	165.148	60.21	2.2477146	7	3	1	0
308	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	0	8	3	4	0	146.106	127.31	2.2290666	6	3	4	0
309	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	0	8	2	0	3	138.619	17.07	1.7991202	7	1	0	1
310	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	0	8	4	2	3	189.171	87.74	2.3757381	11	4	3	0
311	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	0	8	3	1	2	158.201	41.57	2.3260104	14	2	2	0
312	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	0	8	1	0	1	158.559	17.07	2.1120661	4	1	0	2
313	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	0	8	1	0	0	224.348	23.55	2.7142256	24	1	2	0
314	1176	urea	CH4N2O	C(=O)(N)N	0	8	1	2	0	60.056	69.11	1.6403361	4	1	2	0
315	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	0	8	1	0	3	134.178	17.07	2.2423094	10	1	0	0
316	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	0	8	1	0	4	148.205	17.07	2.3420428	12	1	0	0
317	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	0	8	3	1	2	139.11	63.37	2.1552786	5	3	1	0
318	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	0	8	3	0	4	105.093	52.37	1.7991202	7	3	1	0
319	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	0	8	5	0	3	121.048	78.67	1.7988538	3	5	1	0
320	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	0	8	3	0	9	175.228	52.37	2.4078886	17	3	1	0
321	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	0	8	3	0	7	147.174	52.37	2.2378826	13	3	1	0
322	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	0	8	6	0	9	275.197	87.9	2.5331818	14	6	1	0
323	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	0	8	2	0	1	123.111	43.14	2.1120661	5	2	1	0
324	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	0	8	4	1	3	119.076	80.44	2.0170171	5	4	1	0
325	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	0	8	5	1	3	184.107	106.51	2.214052	4	5	2	0
326	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	0	8	3	0	1	190.158	70.08	2.3885948	6	3	2	0
327	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	0	8	3	1	2	138.126	69.16	2.1400209	6	2	2	0
328	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	0	8	2	0	1	260.891	43.14	2.1120661	1	2	1	4
329	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	0	8	3	1	2	207.016	69.16	2.1400209	4	2	2	2
330	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	0	8	4	0	2	168.108	86.28	2.1400209	4	4	2	0
331	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	0	8	2	0	1	249.007	43.14	2.1120661	4	2	1	1
332	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	0	8	7	0	14	290.189	80.29	2.4562006	20	7	0	0
333	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	0	8	4	0	15	266.318	44.76	2.680459	27	4	0	0
334	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	0	8	4	1	5	126.048	55.76	1.7790463	7	4	0	0
335	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	0	8	6	3	7	170.057	104.06	2.2680478	7	6	0	0
336	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	0	8	4	0	9	182.156	44.76	2.1906621	15	4	0	0
337	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	0	8	4	1	19	322.426	55.76	2.9151042	35	4	0	0
338	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	0	8	4	1	7	154.102	55.76	2.114427	11	4	0	0
339	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	0	8	5	3	6	141.063	92.78	2.1606935	8	4	1	0
340	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	0	8	4	3	4	111.037	83.55	2.0205256	6	3	1	0
341	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	0	8	8	1	7	340.184	142.04	2.7103774	9	8	2	0
342	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	0	8	4	2	4	174.092	66.76	2.3859258	7	4	0	0
343	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	0	8	3	0	6	137.095	35.53	1.9512078	10	3	0	0
344	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	0	8	4	2	6	140.075	66.76	2.1466723	9	4	0	0
345	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	0	8	3	0	10	193.203	35.53	2.4183363	18	3	0	0
346	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	0	8	3	2	10	194.211	57.53	2.5804339	19	3	0	0
347	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	0	8	2	0	1	176.624	34.14	2.0946397	5	2	0	1
348	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	0	8	2	1	15	256.43	37.3	2.8959199	32	2	0	0
349	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	0	8	1	0	1	178.615	17.07	2.1120661	4	1	0	2
350	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	0	8	1	0	1	160.625	17.07	2.1120661	5	1	0	1
351	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	1	1	1	1	1	127.574	26.02	2.1120661	6	0	1	1
352	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	1	1	3	1	2	138.126	69.16	2.1311082	6	2	2	0
353	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	1	1	1	1	1	111.119	26.02	2.1120661	6	0	1	1
354	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	1	1	4	1	4	168.152	78.39	2.2222351	8	3	2	0
355	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	1	1	3	1	3	152.153	69.16	2.1964662	8	2	2	0
356	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	1	1	3	1	3	171.221	60.16	2.2423094	9	2	1	0
357	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	1	1	4	1	6	196.206	78.39	2.4160557	12	3	2	0
358	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	1	1	3	1	2	178.235	38.49	2.4591717	14	1	2	0
359	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	1	1	3	1	2	172.571	69.16	2.1837138	5	2	2	1
360	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	1	1	3	1	2	225.191	60.16	2.2423094	6	2	1	3
361	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	1	1	1	1	1	470.817	26.02	2.1120661	4	0	1	3
362	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	1	1	3	1	4	166.18	69.16	2.2238177	10	2	2	0
363	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	1	1	2	1	7	144.214	37.3	2.4325145	16	2	0	0
364	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	1	1	3	2	3	90.078	57.53	1.9894655	6	3	0	0
365	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	1	1	3	2	2	137.138	63.32	2.2585839	7	2	1	0
366	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	1	1	5	4	4	170.12	97.99	2.3720847	6	5	0	0
367	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	1	1	5	2	2	167.12	87.49	2.3315544	5	4	1	0
368	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	1	1	4	3	1	156.097	103.02	2.2319352	4	4	2	0
369	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	1	1	3	2	1	189.17	70.16	2.4576751	7	3	1	0
370	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	1	1	3	1	5	179.219	50.19	2.4790777	13	2	1	0
371	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	1	1	2	0	2	137.138	44.01	2.1129569	7	2	1	0
372	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	1	1	3	2	1	139.11	70.16	2.2319352	5	3	1	0
373	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	1	1	2	1	1	122.127	55.98	2.137382	6	1	2	0
374	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	1	1	1	0	1	106.124	17.07	2.1120661	6	1	0	0
375	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	1	1	3	2	4	214.22	57.53	2.5966697	10	3	0	0
376	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	1	1	7	0	2	322.228	103.81	3.1278468	6	7	0	0
377	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	1	1	3	0	3	165.148	60.21	2.2477146	7	3	1	0
378	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	1	1	3	4	0	146.106	127.31	2.2290666	6	3	4	0
379	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	1	1	2	0	3	138.619	17.07	1.7991202	7	1	0	1
380	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	1	1	4	2	3	189.171	87.74	2.3757381	11	4	3	0
381	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	1	1	3	1	2	158.201	41.57	2.3260104	14	2	2	0
382	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	1	1	1	0	1	158.559	17.07	2.1120661	4	1	0	2
383	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	1	1	1	0	0	224.348	23.55	2.7142256	24	1	2	0
384	1176	urea	CH4N2O	C(=O)(N)N	1	1	1	2	0	60.056	69.11	1.6403361	4	1	2	0
385	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	1	1	1	0	3	134.178	17.07	2.2423094	10	1	0	0
386	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	1	1	1	0	4	148.205	17.07	2.3420428	12	1	0	0
387	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	1	1	3	1	2	139.11	63.37	2.1552786	5	3	1	0
388	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	1	1	3	0	4	105.093	52.37	1.7991202	7	3	1	0
389	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	1	1	5	0	3	121.048	78.67	1.7988538	3	5	1	0
390	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	1	1	3	0	9	175.228	52.37	2.4078886	17	3	1	0
391	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	1	1	3	0	7	147.174	52.37	2.2378826	13	3	1	0
392	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	1	1	6	0	9	275.197	87.9	2.5331818	14	6	1	0
393	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	1	1	2	0	1	123.111	43.14	2.1120661	5	2	1	0
394	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	1	1	4	1	3	119.076	80.44	2.0170171	5	4	1	0
395	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	1	1	5	1	3	184.107	106.51	2.214052	4	5	2	0
396	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	1	1	3	0	1	190.158	70.08	2.3885948	6	3	2	0
397	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	1	1	3	1	2	138.126	69.16	2.1400209	6	2	2	0
398	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	1	1	2	0	1	260.891	43.14	2.1120661	1	2	1	4
399	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	1	1	3	1	2	207.016	69.16	2.1400209	4	2	2	2
400	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	1	1	4	0	2	168.108	86.28	2.1400209	4	4	2	0
401	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	1	1	2	0	1	249.007	43.14	2.1120661	4	2	1	1
402	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	1	1	7	0	14	290.189	80.29	2.4562006	20	7	0	0
403	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	1	1	4	0	15	266.318	44.76	2.680459	27	4	0	0
404	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	1	1	4	1	5	126.048	55.76	1.7790463	7	4	0	0
405	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	1	1	6	3	7	170.057	104.06	2.2680478	7	6	0	0
406	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	1	1	4	0	9	182.156	44.76	2.1906621	15	4	0	0
407	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	1	1	4	1	19	322.426	55.76	2.9151042	35	4	0	0
408	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	1	1	4	1	7	154.102	55.76	2.114427	11	4	0	0
409	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	1	1	5	3	6	141.063	92.78	2.1606935	8	4	1	0
410	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	1	1	4	3	4	111.037	83.55	2.0205256	6	3	1	0
411	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	1	1	8	1	7	340.184	142.04	2.7103774	9	8	2	0
412	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	1	1	4	2	4	174.092	66.76	2.3859258	7	4	0	0
413	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	1	1	3	0	6	137.095	35.53	1.9512078	10	3	0	0
414	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	1	1	4	2	6	140.075	66.76	2.1466723	9	4	0	0
415	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	1	1	3	0	10	193.203	35.53	2.4183363	18	3	0	0
416	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	1	1	3	2	10	194.211	57.53	2.5804339	19	3	0	0
417	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	1	1	2	0	1	176.624	34.14	2.0946397	5	2	0	1
418	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	1	1	2	1	15	256.43	37.3	2.8959199	32	2	0	0
419	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	1	1	1	0	1	178.615	17.07	2.1120661	4	1	0	2
420	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	1	1	1	0	1	160.625	17.07	2.1120661	5	1	0	1
421	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	1	2	1	1	1	127.574	26.02	2.1120661	6	0	1	1
422	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	1	2	3	1	2	138.126	69.16	2.1311082	6	2	2	0
423	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	1	2	1	1	1	111.119	26.02	2.1120661	6	0	1	1
424	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	1	2	4	1	4	168.152	78.39	2.2222351	8	3	2	0
425	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	1	2	3	1	3	152.153	69.16	2.1964662	8	2	2	0
426	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	1	2	3	1	3	171.221	60.16	2.2423094	9	2	1	0
427	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	1	2	4	1	6	196.206	78.39	2.4160557	12	3	2	0
428	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	1	2	3	1	2	178.235	38.49	2.4591717	14	1	2	0
429	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	1	2	3	1	2	172.571	69.16	2.1837138	5	2	2	1
430	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	1	2	3	1	2	225.191	60.16	2.2423094	6	2	1	3
431	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	1	2	1	1	1	470.817	26.02	2.1120661	4	0	1	3
432	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	1	2	3	1	4	166.18	69.16	2.2238177	10	2	2	0
433	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	1	2	2	1	7	144.214	37.3	2.4325145	16	2	0	0
434	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	1	2	3	2	3	90.078	57.53	1.9894655	6	3	0	0
435	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	1	2	3	2	2	137.138	63.32	2.2585839	7	2	1	0
436	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	1	2	5	4	4	170.12	97.99	2.3720847	6	5	0	0
437	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	1	2	5	2	2	167.12	87.49	2.3315544	5	4	1	0
438	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	1	2	4	3	1	156.097	103.02	2.2319352	4	4	2	0
439	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	1	2	3	2	1	189.17	70.16	2.4576751	7	3	1	0
440	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	1	2	3	1	5	179.219	50.19	2.4790777	13	2	1	0
441	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	1	2	2	0	2	137.138	44.01	2.1129569	7	2	1	0

442	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	1	2	3	2	1	139.11	70.16	2.2319352	5	3	1	0
443	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	1	2	2	1	1	122.127	55.98	2.137382	6	1	2	0
444	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	1	2	1	0	1	106.124	17.07	2.1120661	6	1	0	0
445	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	1	2	3	2	4	214.22	57.53	2.5966697	10	3	0	0
446	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	1	2	7	0	2	322.228	103.81	3.1278468	6	7	0	0
447	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	1	2	3	0	3	165.148	60.21	2.2477146	7	3	1	0
448	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	1	2	3	4	0	146.106	127.31	2.2290666	6	3	4	0
449	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	1	2	2	0	3	138.619	17.07	1.7991202	7	1	0	1
450	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	1	2	4	2	3	189.171	87.74	2.3757381	11	4	3	0
451	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	1	2	3	1	2	158.201	41.57	2.3260104	14	2	2	0
452	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	1	2	1	0	1	158.559	17.07	2.1120661	4	1	0	2
453	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	1	2	1	0	0	224.348	23.55	2.7142256	24	1	2	0
454	1176	urea	CH4N2O	C(=O)(N)N	1	2	1	2	0	60.056	69.11	1.6403361	4	1	2	0
455	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	1	2	1	0	3	134.178	17.07	2.2423094	10	1	0	0
456	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	1	2	1	0	4	148.205	17.07	2.3420428	12	1	0	0
457	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	1	2	3	1	2	139.11	63.37	2.1552786	5	3	1	0
458	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	1	2	3	0	4	105.093	52.37	1.7991202	7	3	1	0
459	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	1	2	5	0	3	121.048	78.67	1.7988538	3	5	1	0
460	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	1	2	3	0	9	175.228	52.37	2.4078886	17	3	1	0
461	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	1	2	3	0	7	147.174	52.37	2.2378826	13	3	1	0
462	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	1	2	6	0	9	275.197	87.9	2.5331818	14	6	1	0
463	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	1	2	2	0	1	123.111	43.14	2.1120661	5	2	1	0
464	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	1	2	4	1	3	119.076	80.44	2.0170171	5	4	1	0
465	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	1	2	5	1	3	184.107	106.51	2.214052	4	5	2	0
466	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	1	2	3	0	1	190.158	70.08	2.3885948	6	3	2	0
467	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	1	2	3	1	2	138.126	69.16	2.1400209	6	2	2	0
468	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	1	2	2	0	1	260.891	43.14	2.1120661	1	2	1	4
469	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	1	2	3	1	2	207.016	69.16	2.1400209	4	2	2	2
470	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	1	2	4	0	2	168.108	86.28	2.1400209	4	4	2	0
471	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	1	2	2	0	1	249.007	43.14	2.1120661	4	2	1	1
472	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	1	2	7	0	14	290.189	80.29	2.4562006	20	7	0	0
473	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	1	2	4	0	15	266.318	44.76	2.680459	27	4	0	0
474	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	1	2	4	1	5	126.048	55.76	1.7790463	7	4	0	0
475	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	1	2	6	3	7	170.057	104.06	2.2680478	7	6	0	0
476	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	1	2	4	0	9	182.156	44.76	2.1906621	15	4	0	0
477	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	1	2	4	1	19	322.426	55.76	2.9151042	35	4	0	0
478	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	1	2	4	1	7	154.102	55.76	2.114427	11	4	0	0
479	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	1	2	5	3	6	141.063	92.78	2.1606935	8	4	1	0
480	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	1	2	4	3	4	111.037	83.55	2.0205256	6	3	1	0
481	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	1	2	8	1	7	340.184	142.04	2.7103774	9	8	2	0
482	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	1	2	4	2	4	174.092	66.76	2.3859258	7	4	0	0
483	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	1	2	3	0	6	137.095	35.53	1.9512078	10	3	0	0
484	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	1	2	4	2	6	140.075	66.76	2.1466723	9	4	0	0
485	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	1	2	3	0	10	193.203	35.53	2.4183363	18	3	0	0
486	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	1	2	3	2	10	194.211	57.53	2.5804339	19	3	0	0
487	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	1	2	2	0	1	176.624	34.14	2.0946397	5	2	0	1
488	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	1	2	2	1	15	256.43	37.3	2.8959199	32	2	0	0
489	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	1	2	1	0	1	178.615	17.07	2.1120661	4	1	0	2
490	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	1	2	1	0	1	160.625	17.07	2.1120661	5	1	0	1
491	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	1	4	1	1	1	127.574	26.02	2.1120661	6	0	1	1
492	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	1	4	3	1	2	138.126	69.16	2.1311082	6	2	2	0
493	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	1	4	1	1	1	111.119	26.02	2.1120661	6	0	1	1
494	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	1	4	4	1	4	168.152	78.39	2.2222351	8	3	2	0
495	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	1	4	3	1	3	152.153	69.16	2.1964662	8	2	2	0
496	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	1	4	3	1	3	171.221	60.16	2.2423094	9	2	1	0
497	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	1	4	4	1	6	196.206	78.39	2.4160557	12	3	2	0
498	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	1	4	3	1	2	178.235	38.49	2.4591717	14	1	2	0
499	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	1	4	3	1	2	172.571	69.16	2.1837138	5	2	2	1
500	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	1	4	3	1	2	225.191	60.16	2.2423094	6	2	1	3
501	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	1	4	1	1	1	470.817	26.02	2.1120661	4	0	1	3
502	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	1	4	3	1	4	166.18	69.16	2.2238177	10	2	2	0
503	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	1	4	2	1	7	144.214	37.3	2.4325145	16	2	0	0
504	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	1	4	3	2	3	90.078	57.53	1.9894655	6	3	0	0
505	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	1	4	3	2	2	137.138	63.32	2.2585839	7	2	1	0
506	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	1	4	5	4	4	170.12	97.99	2.3720847	6	5	0	0
507	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	1	4	5	2	2	167.12	87.49	2.3315544	5	4	1	0
508	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	1	4	4	3	1	156.097	103.02	2.2319352	4	4	2	0
509	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	1	4	3	2	1	189.17	70.16	2.4576751	7	3	1	0
510	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	1	4	3	1	5	179.219	50.19	2.4790777	13	2	1	0
511	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	1	4	2	0	2	137.138	44.01	2.1129569	7	2	1	0
512	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	1	4	3	2	1	139.11	70.16	2.2319352	5	3	1	0
513	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	1	4	2	1	1	122.127	55.98	2.137382	6	1	2	0
514	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	1	4	1	0	1	106.124	17.07	2.1120661	6	1	0	0
515	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	1	4	3	2	4	214.22	57.53	2.5966697	10	3	0	0
516	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	1	4	7	0	2	322.228	103.81	3.1278468	6	7	0	0
517	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	1	4	3	0	3	165.148	60.21	2.2477146	7	3	1	0
518	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	1	4	3	4	0	146.106	127.31	2.2290666	6	3	4	0
519	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	1	4	2	0	3	138.619	17.07	1.7991202	7	1	0	1
520	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	1	4	4	2	3	189.171	87.74	2.3757381	11	4	3	0
521	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	1	4	3	1	2	158.201	41.57	2.3260104	14	2	2	0
522	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	1	4	1	0	1	158.559	17.07	2.1120661	4	1	0	2
523	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	1	4	1	0	0	224.348	23.55	2.7142256	24	1	2	0
524	1176	urea	CH4N2O	C(=O)(N)N	1	4	1	2	0	60.056	69.11	1.6403361	4	1	2	0
525	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	1	4	1	0	3	134.178	17.07	2.2423094	10	1	0	0
526	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	1	4	1	0	4	148.205	17.07	2.3420428	12	1	0	0
527	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	1	4	3	1	2	139.11	63.37	2.1552786	5	3	1	0
528	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	1	4	3	0	4	105.093	52.37	1.7991202	7	3	1	0
529	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	1	4	5	0	3	121.048	78.67	1.7988538	3	5	1	0
530	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	1	4	3	0	9	175.228	52.37	2.4078886	17	3	1	0
531	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	1	4	3	0	7	147.174	52.37	2.2378826	13	3	1	0
532	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	1	4	6	0	9	275.197	87.9	2.5331818	14	6	1	0
533	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	1	4	2	0	1	123.111	43.14	2.1120661	5	2	1	0
534	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	1	4	4	1	3	119.076	80.44	2.0170171	5	4	1	0
535	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	1	4	5	1	3	184.107	106.51	2.214052	4	5	2	0
536	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	1	4	3	0	1	190.158	70.08	2.3885948	6	3	2	0
537	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	1	4	3	1	2	138.126	69.16	2.1400209	6	2	2	0
538	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C(=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	1	4	2	0	1	260.891	43.14	2.1120661	1	2	1	4
539	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	1	4	3	1	2	207.016	69.16	2.1400209	4	2	2	2
540	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	1	4	4	0	2	168.108	86.28	2.1400209	4	4	2	0
541	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1[N+](=O)[O-])I	1	4	2	0	1	249.007	43.14	2.1120661	4	2	1	1
542	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	1	4	7	0	14	290.189	80.29	2.4562006	20	7	0	0
543	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	1	4	4	0	15	266.318	44.76	2.680459	27	4	0	0
544	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	1	4	4	1	5	126.048	55.76	1.7790463	7	4	0	0
545	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	1	4	6	3	7	170.057	104.06	2.2680478	7	6	0	0
546	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	1	4	4	0	9	182.156	44.76	2.1906621	15	4	0	0
547	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	1	4	4	1	19	322.426	55.76	2.9151042	35	4	0	0
548	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	1	4	4	1	7	154.102	55.76	2.114427	11	4	0	0
549	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	1	4	5	3	6	141.063	92.78	2.1606935	8	4	1	0
550	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	1	4	4	3	4	111.037	83.55	2.0205256	6	3	1	0
551	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	1	4	8	1	7	340.184	142.04	2.7103774	9	8	2	0
552	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	1	4	4	2	4	174.092	66.76	2.3859258	7	4	0	0
553	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	1	4	3	0	6	137.095	35.53	1.9512078	10	3	0	0
554	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	1	4	4	2	6	140.075	66.76	2.1466723	9	4	0	0
555	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	1	4	3	0	10	193.203	35.53	2.4183363	18	3	0	0
556	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	1	4	3	2	10	194.211	57.53	2.5804339	19	3	0	0
557	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)(=O)Cl	1	4	2	0	1	176.624	34.14	2.0946397	5	2	0	1
558	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	1	4	2	1	15	256.43	37.3	2.8959199	32	2	0	0
559	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	1	4	1	0	1	178.615	17.07	2.1120661	4	1	0	2
560	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	1	4	1	0	1	160.625	17.07	2.1120661	5	1	0	1
561	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	1	6	1	1	1	127.574	26.02	2.1120661	6	0	1	1
562	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)[N+](=O)[O-])N	1	6	3	1	2	138.126	69.16	2.1311082	6	2	2	0
563	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	1	6	1	1	1	111.119	26.02	2.1120661	6	0	1	1
564	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=C(C=C1)[N+](=O)[O-])N	1	6	4	1	4	168.152	78.39	2.2222351	8	3	2	0
565	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	1	6	3	1	3	152.153	69.16	2.1964662	8	2	2	0
566	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	1	6	3	1	3	171.221	60.16	2.2423094	9	2	1	0
567	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	1	6	4	1	6	196.206	78.39	2.4160557	12	3	2	0
568	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	1	6	3	1	2	178.235	38.49	2.4591717	14	1	2	0
569	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	1	6	3	1	2	172.571	69.16	2.1837138	5	2	2	1
570	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	1	6	3	1	2	225.191	60.16	2.2423094	6	2	1	3
571	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	1	6	1	1	1	470.817	26.02	2.1120661	4	0	1	3
572	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	1	6	3	1	4	166.18	69.16	2.2238177	10	2	2	0
573	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	1	6	2	1	7	144.214	37.3	2.4325145	16	2	0	0
574	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	1	6	3	2	3	90.078	57.53	1.9894655	6	3	0	0
575	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	1	6	3	2	2	137.138	63.32	2.2585839	7	2	1	0
576	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	1	6	5	4	4	170.12	97.99	2.3720847	6	5	0	0
577	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	1	6	5	2	2	167.12	87.49	2.3315544	5	4	1	0
578	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	1	6	4	3	1	156.097	103.02	2.2319352	4	4	2	0
579	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	1	6	3	2	1	189.17	70.16	2.4576751	7	3	1	0
580	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	1	6	3	1	5	179.219	50.19	2.4790777	13	2	1	0
581	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	1	6	2	0	2	137.138	44.01	2.1129569	7	2	1	0
582	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	1	6	3	2	1	139.11	70.16	2.2319352	5	3	1	0
583	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	1	6	2	1	1	122.127	55.98	2.137382	6	1	2	0
584	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	1	6	1	0	1	106.124	17.07	2.1120661	6	1	0	0
585	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	1	6	3	2	4	214.22	57.53	2.5966697	10	3	0	0
586	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	1	6	7	0	2	322.228	103.81	3.1278468	6	7	0	0
587	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	1	6	3	0	3	165.148	60.21	2.2477146	7	3	1	0
588	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	1	6	3	4	0	146.106	127.31	2.2290666	6	3	4	0

589	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	1	6	2	0	3	138.619	17.07	1.7991202	7	1	0	1
590	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	1	6	4	2	3	189.171	87.74	2.3757381	11	4	3	0
591	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	1	6	3	1	2	158.201	41.57	2.3260104	14	2	2	0
592	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	1	6	1	0	1	158.559	17.07	2.1120661	4	1	0	2
593	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	1	6	1	0	0	224.348	23.55	2.7142256	24	1	2	0
594	1176	urea	CH4N2O	C(=O)(N)N	1	6	1	2	0	60.056	69.11	1.6403361	4	1	2	0
595	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	1	6	1	0	3	134.178	17.07	2.2423094	10	1	0	0
596	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	1	6	1	0	4	148.205	17.07	2.3420428	12	1	0	0
597	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	1	6	3	1	2	139.11	63.37	2.1552786	5	3	1	0
598	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	1	6	3	0	4	105.093	52.37	1.7991202	7	3	1	0
599	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	1	6	5	0	3	121.048	78.67	1.7988538	3	5	1	0
600	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCCC(CO[N+](=O)[O-]	1	6	3	0	9	175.228	52.37	2.4078886	17	3	1	0
601	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	1	6	3	0	7	147.174	52.37	2.2378826	13	3	1	0
602	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	1	6	6	0	9	275.197	87.9	2.5331818	14	6	1	0
603	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	1	6	2	0	1	123.111	43.14	2.1120661	5	2	1	0
604	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	1	6	4	1	3	119.076	80.44	2.0170171	5	4	1	0
605	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	1	6	5	1	3	184.107	106.51	2.214052	4	5	2	0
606	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	1	6	3	0	1	190.158	70.08	2.3885948	6	3	2	0
607	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	1	6	3	1	2	138.126	69.16	2.1400209	6	2	2	0
608	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	1	6	2	0	1	260.891	43.14	2.1120661	1	2	1	4
609	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	1	6	3	1	2	207.016	69.16	2.1400209	4	2	2	2
610	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	1	6	4	0	2	168.108	86.28	2.1400209	4	4	2	0
611	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1I)[N+](=O)[O-])I	1	6	2	0	1	249.007	43.14	2.1120661	4	2	1	1
612	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	1	6	7	0	14	290.189	80.29	2.4562006	20	7	0	0
613	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	1	6	4	0	15	266.318	44.76	2.680459	27	4	0	0
614	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	1	6	4	1	5	126.048	55.76	1.7790463	7	4	0	0
615	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	1	6	6	3	7	170.057	104.06	2.2680478	7	6	0	0
616	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	1	6	4	0	9	182.156	44.76	2.1906621	15	4	0	0
617	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	1	6	4	1	19	322.426	55.76	2.9151042	35	4	0	0
618	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	1	6	4	1	7	154.102	55.76	2.114427	11	4	0	0
619	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	1	6	5	3	6	141.063	92.78	2.1606935	8	4	1	0
620	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	1	6	4	3	4	111.037	83.55	2.0205256	6	3	1	0
621	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	1	6	8	1	7	340.184	142.04	2.7103774	9	8	2	0
622	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	1	6	4	2	4	174.092	66.76	2.3859258	7	4	0	0
623	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	1	6	3	0	6	137.095	35.53	1.9512078	10	3	0	0
624	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	1	6	4	2	6	140.075	66.76	2.1466723	9	4	0	0
625	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	1	6	3	0	10	193.203	35.53	2.4183363	18	3	0	0
626	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	1	6	3	2	10	194.211	57.53	2.5804339	19	3	0	0
627	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)=O)Cl	1	6	2	0	1	176.624	34.14	2.0946397	5	2	0	1
628	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	1	6	2	1	15	256.43	37.3	2.8959199	32	2	0	0
629	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	1	6	1	0	1	178.615	17.07	2.1120661	4	1	0	2
630	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	1	6	1	0	1	160.625	17.07	2.1120661	5	1	0	1
631	7812	4-chloroaniline	C6H6ClN	C1=CC(=CC=C1N)Cl	1	8	1	1	1	127.574	26.02	2.1120661	6	0	1	1
632	7423	3-nitroaniline	C6H6N2O2	C1=CC(=CC(=C1)N)[N+](=O)[O-])N	1	8	3	1	2	138.126	69.16	2.1311082	6	2	2	0
633	9731	4-fluoroaniline	C6H6FN	C1=CC(=CC=C1N)F	1	8	1	1	1	111.119	26.02	2.1120661	6	0	1	1
634	7447	2-methoxy-5-nitroaniline	C7H8N2O3	COC1=C(C=CC(=C1)[N+](=O)[O-])N	1	8	4	1	4	168.152	78.39	2.2222351	8	3	2	0
635	7441	2-methyl-4-nitroaniline	C7H8N2O2	CC1=C(C=CC(=C1)[N+](=O)[O-])N	1	8	3	1	3	152.153	69.16	2.1964662	8	2	2	0
636	79617	4-methylsulfonylaniline	C7H9NO2S	CS(=O)(=O)C1=CC=C(C=C1)N	1	8	3	1	3	171.221	60.16	2.2423094	9	2	1	0
637	11118	5-nitro-2-propoxyaniline	C9H12N2O3	CCCOC1=C(C=C(C=C1)[N+](=O)[O-])N	1	8	4	1	6	196.206	78.39	2.4160557	12	3	2	0
638	75655	4-morpholin-4-ylaniline	C10H14N2O	C1COCCN1C2=CC=C(C=C2)N	1	8	3	1	2	178.235	38.49	2.4591717	14	1	2	0
639	74218	5-chloro-2-nitroaniline	C6H5ClN2O2	C1=CC(=C(C=C1Cl)N)[N+](=O)[O-]	1	8	3	1	2	172.571	69.16	2.1837138	5	2	2	1
640	136315	4-(trifluoromethylsulfonyl)aniline	C7H6F3NO2S	C1=CC(=CC=C1N)S(=O)(=O)C(F)(F)F	1	8	3	1	2	225.191	60.16	2.2423094	6	2	1	3
641	222556	2,4,6-triiodoaniline	C6H4I3N	C1=C(C=C(C(=C1I)N)I)I	1	8	1	1	1	470.817	26.02	2.1120661	4	0	1	3
642	28159	2,6-dimethyl-4-nitroaniline	C8H10N2O2	CC1=CC(=CC(=C1N)C)[N+](=O)[O-]	1	8	3	1	4	166.18	69.16	2.2238177	10	2	2	0
643	379	octanoic acid	C8H16O2	CCCCCCCC(=O)O	1	8	2	1	7	144.214	37.3	2.4325145	16	2	0	0
644	612	2-hydroxypropanoic acid	C3H6O3	CC(C(=O)O)O	1	8	3	2	3	90.078	57.53	1.9894655	6	3	0	0
645	978	4-aminobenzoic acid	C7H7NO2	C1=CC(=CC=C1C(=O)O)N	1	8	3	2	2	137.138	63.32	2.2585839	7	2	1	0
646	370	3,4,5-trihydroxybenzoic acid	C7H6O5	C1=C(C=C(C(=C1O)O)O)C(=O)O	1	8	5	4	4	170.12	97.99	2.3720847	6	5	0	0
647	1066	pyridine-2,3-dicarboxylic acid	C7H5NO4	C1=CC(=C(N=C1)C(=O)O)C(=O)O	1	8	5	2	2	167.12	87.49	2.3315544	5	4	1	0
648	967	2,4-dioxo-1H-pyrimidine-6-carboxylic acid	C5H4N2O4	C1=C(NC(=O)NC1=O)C(=O)O	1	8	4	3	1	156.097	103.02	2.2319352	4	4	2	0
649	3845	4-oxo-1H-quinoline-2-carboxylic acid	C10H7NO3	C1=CC=C2C(=C1)C(=O)C=C(N2)C(=O)O	1	8	3	2	1	189.17	70.16	2.4576751	7	3	1	0
650	3442	5-butylpyridine-2-carboxylic acid	C10H13NO2	CCCCC1=CN=C(C=C1)C(=O)O	1	8	3	1	5	179.219	50.19	2.4790777	13	2	1	0
651	5570	1-methylpyridin-1-ium-3-carboxylate	C7H7NO2	C[N+]1=CC=CC(=C1)C(=O)[O-]	1	8	2	0	2	137.138	44.01	2.1129569	7	2	1	0
652	72924	6-oxo-1H-pyridine-3-carboxylic acid	C6H5NO3	C1=CC(=O)NC=C1C(=O)O	1	8	3	2	1	139.11	70.16	2.2319352	5	3	1	0
653	936	pyridine-3-carboxamide	C6H6N2O	C1=CC(=CN=C1)C(=O)N	1	8	2	1	1	122.127	55.98	2.137382	6	1	2	0
654	240	benzaldehyde	C7H6O	C1=CC=C(C=C1)C=O	1	8	1	0	1	106.124	17.07	2.1120661	6	1	0	0
655	69150	bis(4-hydroxyphenyl)methanone	C13H10O3	C1=CC(=CC=C1C(=O)C2=CC=C(C=C2)O)O	1	8	3	2	4	214.22	57.53	2.5966697	10	3	0	0
656	75498	5-(1,3-dioxo-2-benzofuran-5-carbonyl)-2-benzofuran-1,3-dione	C17H6O7	C1=CC2=C(C=C1C(=O)C3=CC4=C(C=C3)C(=O)OC4=O)C(=O)OC2=O	1	8	7	0	2	322.228	103.81	3.1278468	6	7	0	0
657	7487	1-(4-nitrophenyl)ethanone	C8H7NO3	CC(=O)C1=CC=C(C=C1)[N+](=O)[O-]	1	8	3	0	3	165.148	60.21	2.2477146	7	3	1	0
658	68400	1,3-dicarbamoylurea	C3H6N4O3	C(=O)(N)NC(=O)NC(=O)N	1	8	3	4	0	146.106	127.31	2.2260666	6	3	4	0
659	26323	S-propyl chloromethanethioate	C4H7ClOS	CCCSC(=O)Cl	1	8	2	0	3	138.619	17.07	1.7991202	7	1	0	1
660	54747	[acetyl(methylcarbamoyl)amino] N-methylcarbamate	C6H11N3O4	CC(=O)N(C(=O)NC)OC(=O)NC	1	8	4	2	3	189.171	87.74	2.3757381	11	4	3	0
661	8431	ethyl piperazine-1-carboxylate	C7H14N2O2	CCOC(=O)N1CCNCC1	1	8	3	1	2	158.201	41.57	2.3260104	14	2	2	0
662	9808	2-fluorobenzoyl chloride	C7H4ClFO	C1=CC=C(C(=C1)C(=O)Cl)F	1	8	1	0	1	158.559	17.07	2.1120661	4	1	0	2
663	160117	bis(azepan-1-yl)methanone	C13H24N2O	C1CCCN(CC1)C(=O)N2CCCCCC2	1	8	1	0	0	224.348	23.55	2.7142256	24	1	2	0
664	1176	urea	CH4N2O	C(=O)(N)N	1	8	1	2	0	60.056	69.11	1.6403361	4	1	2	0
665	20861	4-ethylbenzaldehyde	C9H10O	CCC1=CC=C(C=C1)C=O	1	8	1	0	3	134.178	17.07	2.2423094	10	1	0	0
666	120047	4-propylbenzaldehyde	C10H12O	CCCC1=CC=C(C=C1)C=O	1	8	1	0	4	148.205	17.07	2.3420428	12	1	0	0
667	980	4-nitrophenol	C6H5NO3	C1=CC(=CC=C1[N+](=O)[O-])O	1	8	3	1	2	139.11	63.37	2.1552786	5	3	1	0
668	12307	propyl nitrate	C3H7NO3	CCCO[N+](=O)[O-]	1	8	3	0	4	105.093	52.37	1.7991202	7	3	1	0
669	16782	nitro ethaneperoxoate	C2H3NO5	CC(=O)OO[N+](=O)[O-]	1	8	5	0	3	121.048	78.67	1.7988538	3	5	1	0
670	62823	2-ethylhexyl nitrate	C8H17NO3	CCCCC(CC)CO[N+](=O)[O-]	1	8	3	0	9	175.228	52.37	2.4078886	17	3	1	0
671	30209	hexyl nitrate	C6H13NO3	CCCCCCO[N+](=O)[O-]	1	8	3	0	7	147.174	52.37	2.2378826	13	3	1	0
672	9395	diethyl (4-nitrophenyl) phosphate	C10H14NO6P	CCOP(=O)(OCC)OC1=CC=C(C=C1)[N+](=O)[O-]	1	8	6	0	9	275.197	87.9	2.5331818	14	6	1	0
673	7416	nitrobenzene	C6H5NO2	C1=CC=C(C=C1)[N+](=O)[O-]	1	8	2	0	1	123.111	43.14	2.1120661	5	2	1	0
674	1678	3-nitropropanoic acid	C3H5NO4	C(C[N+](=O)[O-])C(=O)O	1	8	4	1	3	119.076	80.44	2.0170171	5	4	1	0
675	1493	2,4-dinitrophenol	C6H4N2O5	C1=CC(=C(C=C1[N+](=O)[O-])[N+](=O)[O-])O	1	8	5	1	3	184.107	106.51	2.214052	4	5	2	0
676	5955	4-nitro-1-oxidoquinolin-1-ium	C9H6N2O3	C1=CC=C2C(=C1)C(=CC=[N+]2[O-])[N+](=O)[O-]	1	8	3	0	1	190.158	70.08	2.3885948	6	3	2	0
677	7475	4-nitroaniline	C6H6N2O2	C1=CC(=CC=C1N)[N+](=O)[O-]	1	8	3	1	2	138.126	69.16	2.1400209	6	2	2	0
678	8330	1,2,4,5-tetrachloro-3-nitrobenzene	C6HCl4NO2	C1=C(C=C(C(=C1Cl)Cl)[N+](=O)[O-])Cl)Cl	1	8	2	0	1	260.891	43.14	2.1120661	1	2	1	4
679	7430	2,6-dichloro-4-nitroaniline	C6H4Cl2N2O2	C1=C(C=C(C(=C1Cl)N)Cl)[N+](=O)[O-]	1	8	3	1	2	207.016	69.16	2.1400209	4	2	2	2
680	7492	1,4-dinitrobenzene	C6H4N2O4	C1=CC(=CC=C1[N+](=O)[O-])[N+](=O)[O-]	1	8	4	0	2	168.108	86.28	2.1400209	4	4	2	0
681	12495	1-iodo-4-nitrobenzene	C6H4INO2	C1=CC(=CC=C1I)[N+](=O)[O-])I	1	8	2	0	1	249.007	43.14	2.1120661	4	2	1	1
682	7873	diethoxyphosphoryl diethyl phosphate	C8H20O7P2	CCOP(=O)(OCC)OP(=O)(OCC)OCC	1	8	7	0	14	290.189	80.29	2.4562006	20	7	0	0
683	31357	tributyl phosphate	C12H27O4P	CCCCOP(=O)(OCCCC)OCCCC	1	8	4	0	15	266.318	44.76	2.680459	27	4	0	0
684	13134	dimethyl hydrogen phosphate	C2H7O4P	COP(=O)(O)OC	1	8	4	1	5	126.048	55.76	1.7790463	7	4	0	0
685	668	(3-hydroxy-2-oxopropyl) dihydrogen phosphate	C3H7O6P	C(C(=O)COP(=O)(O)O)O	1	8	6	3	7	170.057	104.06	2.2680478	7	6	0	0
686	6535	triethyl phosphate	C6H15O4P	CCOP(=O)(OCC)OCC	1	8	4	0	9	182.156	44.76	2.1906621	15	4	0	0
687	9275	bis(2-ethylhexyl) hydrogen phosphate	C16H35O4P	CCCCC(CC)COP(=O)(O)OCC(CC)CCCC	1	8	4	1	19	322.426	55.76	2.9151042	35	4	0	0
688	654	diethyl hydrogen phosphate	C4H11O4P	CCOP(=O)(O)OCC	1	8	4	1	7	154.102	55.76	2.114427	11	4	0	0
689	1015	2-aminoethyl dihydrogen phosphate	C2H8NO4P	C(COP(=O)(O)O)N	1	8	5	3	6	141.063	92.78	2.1606935	8	4	1	0
690	14017	aminomethylphosphonic acid	CH6NO3P	C(N)P(=O)(O)O	1	8	4	3	4	111.037	83.55	2.0205256	6	3	1	0
691	255	bis(4-nitrophenyl) hydrogen phosphate	C12H9N2O8P	C1=CC(=CC=C1[N+](=O)[O-])OP(=O)(O)OC2=CC=C(C=C2)[N+](=O)[O-]	1	8	8	1	7	340.184	142.04	2.7103774	9	8	2	0
692	12793	phenyl dihydrogen phosphate	C6H7O4P	C1=CC=C(C=C1)OP(=O)(O)O	1	8	4	2	4	174.092	66.76	2.3859258	7	4	0	0
693	6327654	diethoxy(oxo)phosphanium	C4H10O3P+	CCO[P+](=O)OCC	1	8	3	0	6	137.095	35.53	1.9512078	10	3	0	0
694	74188	propyl dihydrogen phosphate	C3H9O4P	CCCOP(=O)(O)O	1	8	4	2	6	140.075	66.76	2.1466723	9	4	0	0
695	6327349	dibutoxy(oxo)phosphanium	C8H18O3P+	CCCCO[P+](=O)OCCCC	1	8	3	0	10	193.203	35.53	2.4183363	18	3	0	0
696	78452	octylphosphonic acid	C8H19O3P	CCCCCCCCP(=O)(O)O	1	8	3	2	10	194.211	57.53	2.5804339	19	3	0	0
697	7369	benzenesulfonyl chloride	C6H5ClO2S	C1=CC=C(C=C1)S(=O)=O)Cl	1	8	2	0	1	176.624	34.14	2.0946397	5	2	0	1
698	985	hexadecanoic acid	C16H32O2	CCCCCCCCCCCCCCCC(=O)O	1	8	2	1	15	256.43	37.3	2.8959199	32	2	0	0
699	12669616	4-fluorobenzenesulfinyl chloride	C6H4ClFOS	C1=CC(=CC=C1F)S(=O)Cl	1	8	1	0	1	178.615	17.07	2.1120661	4	1	0	2
700	4190003	benzenesulfinyl chloride	C6H5ClOS	C1=CC=C(C=C1)S(=O)Cl	1	8	1	0	1	160.625	17.07	2.1120661	5	1	0	1