

Supporting Information  
For  
Computer-Aided Molecular Design and Selection  
of CO<sub>2</sub> Capture Solvents Considering  
Thermodynamics, Reactivity and Sustainability

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## Table of Contents

<b>Section A: Heuristics for the identification of CO<sub>2</sub> chemisorption solvents.....</b>	S3
<b>Section B: Calculation methods.....</b>	S4
<b>Section C: Calculating EHS and LCA metrics .....</b>	S7
<b>Section D: The SAFT-<math>\gamma</math> SW model .....</b>	S11
<b>Section E: Data for reported solvents .....</b>	S14
<b>Section F: Assessment of the 29 solvents selected from the databases (Classes C and R) .....</b>	S20
<b>Cited References .....</b>	S24

## Section A: Heuristics for the identification of CO<sub>2</sub> chemisorption solvents

Selected rules-of-thumb to identify promising molecular structures for CO<sub>2</sub> capture are listed in Table 1 and explained in this section.

**Structure-Property Relation (1)** relates to the number of carbon atoms that separate amine and hydroxyl groups for high absorption capacity. Following the experimental screening of 76 amines, Puxty et al.<sup>1</sup> found that those with outstanding CO<sub>2</sub> absorption capacities shared several structural features, including hydroxyl functionality two or three carbons away from the amine nitrogen. Yamada et al.<sup>2</sup> also observed that the CO<sub>2</sub> loading increases as the number of carbon atoms between the hydroxyl and the amine nitrogen increase from two to four, with a considerably higher increase from two to three carbon atoms. Hydroxylamines with similar structural characteristics are also proposed in Tontiwachwuthikul et al.<sup>3</sup> as options that enable high CO<sub>2</sub> absorption capacity and low regeneration energy.

**Structure-Property Relation (2)** is based on observations by Aronu et al.<sup>4</sup> that increased chain length between the amine functional groups increases basicity and by Singh and Versteeg<sup>5</sup> that in linear diamines, the desorption capacity increases with increasing separation between the amine groups, up to 6 carbon atoms.

**Structure-Property Relation (3)** indicates that desorption is favoured when a hydroxyl group is present and attached the  $\beta$ -carbon atom (with respect to the amine nitrogen) rather than to the  $\alpha$ -carbon as found by Singh and Versteeg<sup>5</sup> and Singh et al.<sup>6, 7</sup>. The authors conclude, however, that the increase in desorption capacity is associated with a decrease in absorption capacity, which contradicts the ON rule, highlighting the challenges inherent in qualitative rules. In diamines, a similar impact on the desorption capacity is observed when the second amine group appears as a branch from the  $\beta$ -carbon atom relative to the first amine group<sup>5</sup>.

**Structure-Property Relation (4)** indicates that, in the case of linear hydroxylamines, an improved desorption capacity is observed in chains of up to 4 carbon atoms, as the chain length increases<sup>5</sup>.

**Structure-Property Relation (5)** is based on the observation by Zhang et al.<sup>8</sup> that the presence of an alkyl branch in an alkylamine at the  $\beta$ -carbon (with respect to the amine) leads to unwanted bicarbonate precipitation but that branching at an  $\alpha$ -carbon has a positive influence on kinetics.

**Structure-Property Relation (6): Steric hindrance** is a property affecting both the absorption rate and capacity of the solvent. It is associated with the ability of amines to form stable carbamates and affects the amine-CO<sub>2</sub> reaction stoichiometry<sup>9</sup>. In unhindered amines that form stable carbamates the reaction stoichiometry allows for 0.5 mol CO<sub>2</sub> to be absorbed per mole of amine, while in hindered amines this increases to 1 mol CO<sub>2</sub>/mol amine. Steric hindrance is associated with the bulkiness of the substituents attached to the amine group in the molecule. Bulky substituents prohibit CO<sub>2</sub> from reaching the reaction centre hence reducing the reaction rate<sup>10</sup>. Sartori et al.<sup>9</sup> suggested that hindered amines have the following characteristics:

- a primary amine is hindered when the amino group is attached to a tertiary carbon;
- a secondary amine is hindered when the amino group is attached to at least one secondary or tertiary carbon.

A detailed investigation of hindered amines in recent work<sup>11</sup> concluded that they conform to these rules. While there exist methods to calculate parameters related to steric hindrance, such as Taft's steric effect parameter  $\Sigma E_s$ <sup>12</sup>, and the topological steric effect index<sup>10</sup>, they have limited applicability to our current work due to the lack of  $\Sigma E_s$  values for many of the substituents<sup>13</sup>.

## Section B: Calculation methods

### B.1 Scaling of properties

In step 1.2 (section 2.1.2) a scaled value  $x_{i,l_j}^*$  of property  $j$  for this solvent obtained using model  $l_j$  is derived as follows:

$$x_{i,l_j}^* = \frac{x_{i,l_j}}{\max_{q \in G} \{ |x_{q,l_j}| \}}, \quad (B1)$$

where  $x_{i,l_j}$  is given by:

$$x_{i,l_j} = \frac{x_{i,l_j} - \mu_{l_j}^G}{s t_{l_j}^G}, \quad (B2)$$

where  $x_{i,l_j}$  represents the value of property  $j$  for molecule  $i$  computed with model  $l_j$ , and  $\mu_{l_j}^G$  and  $s t_{l_j}^G$  represent the mean and standard deviation, respectively, of the property computed with model  $l_j$ , as calculated over the entire set of solvents  $G$ . The standardization scheme applied in equations (B1) and (B2) helps to give equal importance to each property.

In step 2.1 (section 2.2.1) the term  $x_{i,j}^{ave}$  is calculated as follows:

$$x_{i,j}^{ave} = \frac{1}{N_j^{md}} \sum_{l_j=1}^{N_j^{md}} \frac{x_{i,l_j}}{\max_{q \in G} \{ |x_{q,l_j}| \}}. \quad (B3)$$

### B.2 Comments on the uncertainty analysis approach

In principle, the outcome of the distribution of ranks may be sensitive to the number of models utilized to predict each property. It would be especially important to use a large number of models if the frequency of appearance of each solvent in the top positions were used as a final solvent selection criterion. In our work, however, the main objective is to facilitate the appearance at the high-performance end of solvents with even a moderate frequency, and to generate from this an overall solvent set which may be easily reviewed and analyzed.

Similarly, we note that uncertainty is not considered in Step 1.1. This may bias the screening procedure and may lead to some potentially high performance solvents being discarded prematurely. Nevertheless, the approach enables the fast identification of solvents with favourable trade-offs among the numerous properties used as performance criteria, while avoiding options with obviously poor performance. This Pareto optimality conditions lead to a few solvents with properties that cover a wide performance spectrum. In this sense, the multi-

objective CAMD approach serves as a sampling procedure that captures a reduced but sufficiently representative set of high-performance solvents.

### B.3 Models used for calculations and uncertainty analysis in Stage 1

**Table B1:** Models used to evaluate the thermodynamic, reactivity and sustainability property criteria in Stage 1.  $j$  denotes the property number,  $N_j^{md}$  the number of property models used for property  $j$ , “No.” the model number and “Description” indicates the source of the model and the auxiliary properties required as input to the model (cf. Table B2).

$j$	Property	$N_j^{md}$	Models	
			No.	Description
1	Relative energy difference, $RED$	2	1.1	$\delta_1$
			1.2	$\delta_2$
2	Vapour pressure, $P_{vp}$	3	2.1	Riedel correlation <sup>14</sup> + $T_{c,1} + P_{c,1} + T_{b,1}$
			2.2	Riedel correlation <sup>14</sup> + $T_{c,2} + P_{c,2} + T_{b,2}$
			2.3	Wisniak et al. <sup>15</sup> + $T_{c,1} + P_{c,1} + T_{b,1} + \omega$
3	Heat capacity, $C_p$	1	3.1	Rayer et al. <sup>16</sup>
4	Density, $\rho$	2	4.1	$1/V_{m,1}$
			4.2	$1/V_{m,2}$
5	Surface tension, $\sigma$	7	5.1	Conte et al. <sup>17</sup>
			5.2	Sheldon et al. <sup>18</sup> + $V_{m,1} + \delta_1$
			5.3	Sheldon et al. <sup>18</sup> + $V_{m,1} + \delta_2$
			5.4	Sheldon et al. <sup>18</sup> + $V_{m,1} + \delta_3$
			5.5	Sheldon et al. <sup>18</sup> + $V_{m,2} + \delta_1$
6	Viscosity, $n$	3	5.6	Sheldon et al. <sup>18</sup> + $V_{m,2} + \delta_2$
			5.7	Sheldon et al. <sup>18</sup> + $V_{m,2} + \delta_3$
7	Normal melting point, $T_m$	1	6.1	Conte et al. <sup>17</sup>
			6.2	Sastri and Rao <sup>19</sup> + $T_{b,1}$
			6.3	Sastri and Rao <sup>19</sup> + $T_{b,2}$
8	Normal boiling point, $T_b$	1	7.1	Average from Marrero and Gani <sup>20</sup> and Hukkerikar et al. <sup>21</sup>
9	Basicity, $pKa$	1	8.1	Average from Marrero and Gani <sup>20</sup> and Hukkerikar et al. <sup>21</sup>
10	Cumulative energy demand, $CED$	1	9.1	Marvin 6.0.5 <sup>22</sup>
11	Global warming potential, $GWP$	1	10.1	Ecoinvent or FineChem <sup>23</sup>
12	Eco-Indicator-99, $EI99$	1	11.1	Ecoinvent or FineChem <sup>23</sup>
13	Health, safety, and environmental impact index, $EHS$	1	12.1	Ecoinvent or FineChem <sup>23</sup>
			13.1	Cf. Table C4 in Section C

**Table B2:** Auxiliary properties used as input to the models of the property criteria applied to CO<sub>2</sub> capture (cf. Table B1).

Property	Symbol	Source
Critical temperature	$T_{c,1}$	Hukkerikar et al. <sup>21</sup>
Critical temperature	$T_{c,2}$	Marrero and Gani <sup>20</sup>
Critical pressure	$P_{c,1}$	Hukkerikar et al. <sup>21</sup>
Critical pressure	$P_{c,2}$	Marrero and Gani <sup>20</sup>
Normal boiling point	$T_{b,1}$	Hukkerikar et al. <sup>21</sup>
Normal boiling point	$T_{b,2}$	Marrero and Gani <sup>20</sup>
Acentric factor	$\Omega$	Hukkerikar et al. <sup>21</sup>
Molar volume	$V_{m,1}$	Hukkerikar et al. <sup>20</sup>
Molar volume	$V_{m,2}$	Constantinou et al. <sup>24</sup>
Hansen solubility parameter	$\delta_1$	Hukkerikar et al. <sup>21</sup>
Hansen solubility parameter	$\delta_2$	Stefanis and Panayiotou <sup>25</sup>
Hildebrand solubility parameter	$\delta_3$	Sheldon et al. <sup>4</sup>

#### B.4. Calculation of the *RED* index

Hansen<sup>26</sup> divided the solubility parameter into three partial solubility parameters (HSPs), namely the dispersion cohesive energy density HSP ( $\delta_d$ ), the polar cohesive energy density HSP ( $\delta_p$ ), and the hydrogen bonding cohesive energy density HSP ( $\delta_h$ ). This partitioning enables the separate consideration of polar and non-polar interactions. The total Hansen solubility parameter is defined as follows:

$$\delta_t = \sqrt{\delta_d^2 + \delta_p^2 + \delta_h^2}. \quad (\text{B4})$$

Furthermore, the ability of a solvent (B) to dissolve a solute (A) is calculated based on the distance measure  $R_a$  as follows<sup>25</sup>:

$$R_a^2 = 4 \left( \delta_{d,A} - \delta_{d,B} \right)^2 + \left( \delta_{p,A} - \delta_{p,B} \right)^2 + \left( \delta_{h,A} - \delta_{h,B} \right)^2. \quad (\text{B5})$$

This equation can be used in the so-called relative energy difference (*RED*) number<sup>25</sup> as follows:

$$RED = \frac{R_a}{R_0}, \quad (\text{B6})$$

where  $R_0$  is the radius of a Hansen solubility parameter sphere that provides an acceptable distance for the solute of interest<sup>25, 27</sup>. According to Retief<sup>28</sup>, the  $R_0$  value for CO<sub>2</sub> is 3.3 MPa<sup>0.5</sup>, while for A = CO<sub>2</sub> in equation (B5) the values are  $\delta_{d,A} = 15.7$  MPa<sup>0.5</sup>,  $\delta_{p,A} = 5.2$  MPa<sup>0.5</sup>,  $\delta_{h,A} = 5.8$  MPa<sup>0.5</sup>.

## Section C: Calculating EHS and LCA metrics

The scores for the characteristic dangerous properties are calculated based on empirically-derived scales of parameters such as flash points, boiling points, toxicity classification schemes, lethal doses and concentrations, half-lives, octanol/water partitioning coefficients. Sugiyama et al.<sup>29</sup> updated the method with respect to the dangerous property priorities, and considered scaling and scoring methods. The assessment is designed to use pure component properties, since mixture hazard properties are composition specific and both data and reliable estimation models are largely unavailable. Solvent properties are collected from material safety data sheets whenever possible and Quantitative Structure Activity Relationships (QSARs) are used to fill some of the data gaps. The Estimation Program Interface (EPI) Suite<sup>30</sup> and the Toxicity Estimation Software Tool (TEST)<sup>31</sup> developed by the US Environmental Protection Agency are used in that respect. An average of the dangerous properties calculated by the EHS method versions is used to avoid missing scores in the case of persisting data gaps. The EHS score is the sum of the safety, health and environmental scores.

Tables C1 to C3 present in detail the data for the LCA and EHS metrics used in solvent selection and Table C4 refers to the respective data sources for the EHS assessment. Most estimation methods for the EHS categories and the FineChem<sup>23</sup> tool for LCA metrics require the molecular structure and group connectivity to be determined in advance and represented in Simplified Molecular Input Line Entry System (SMILES). However, the relation between the SMILES and the set of molecular structure according to the CAMD procedure is not an injective function, namely more than one SMILES can relate to the same molecular descriptors of the CAMD algorithm. Therefore, in the Design Problem, an algorithm was developed to randomly combine the different molecular descriptors representing a new molecule and create a maximum of 100 feasible, unique SMILES per set of descriptors. The required properties were then estimated for the set of SMILES and averaged to represent the value of the respective CAMD derived molecular structure.

**Table C1(a):** LCA metrics as predicted by the FineChem<sup>23</sup> tool for the solvents of Figure 3.

LCA metrics	1M2P	DPE	4A2B	3DAP	ND1B	1EDB	2P12P	4AP	4D1B
CED (MJ-eq/kg)	106.1	93.5	93.5	108.1	107.4	106.1	165.9	106.7	93.5
GWP (kg CO <sub>2</sub> -eq/kg)	3.4	3.6	3.6	3.2	3.3	3.4	9.6	3.4	3.6
EI-99 (pt/kg)	0.22	0.30	0.30	0.24	0.23	0.22	0.83	0.23	0.30

**Table C1(b):** EHS index values and their decomposition into safety, health and environment categories, dangerous property indices (DPI) and related primary properties (PP) for the solvents of Figure 3 (e.g., the indicator “boiling point” is used to derive the value of the dangerous property called “mobility”).

Primary and Dangerous properties		1M2P	DPE	4A2B	3DAP	ND1B	1EDB	2P12P	4AP	4D1B
PP	Boiling point (°C)	141	144	144	196	176	167	150	180	139
DPI	Mobility	0.53	0.51	0.51	0.30	0.38	0.42	0.49	0.37	0.53
PP	Flashpoint (°C)	73	30	27	69	60	73	33	83	21
DPI	Flammability	0.86	0.96	0.97	0.81	0.86	0.83	0.95	0.79	0.98
PP	LD50oral (mg/kg)	3167	258	326	1581	1150	3835	764	2739	409
DPI	Acute toxicity	0.11	0.38	0.36	0.00	0.08	0.00	0.24	0.00	0.35
PP	Oxygen balance (%)	-224.36	-315.67	-315.67	-262.15	-252.57	-224.36	-288.36	-240.38	-315.67
DPI	Reaction/ Decomposition	0.14	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.00
PP	PH	12.09	12.41	12.29	11.99	11.89	12.05	12.11	12.19	12.27
DPI	Irritation	0.86	0.93	0.90	0.72	0.73	0.79	0.84	0.80	0.90
PP	PP	0.11	0.38	0.36	0.00	0.08	0.00	0.24	0.00	0.35
DPI	Chronic toxicity	0.07	0.29	0.26	0.00	0.02	0.00	0.17	0.00	0.27
PP	Persistency (days)	24	20	13	23	23	25	48	25	28
DPI	Environmental Degradation	0.69	0.65	0.55	0.68	0.68	0.70	0.84	0.70	0.72
PP	LC50aq(mg/l) Water	195	72	74	148	159	273	160	96	54
DPI	mediated effects	0.10	0.20	0.17	0.13	0.12	0.07	0.16	0.18	0.25
PP	Chronic toxicity	0.07	0.29	0.26	0.00	0.02	0.00	0.17	0.00	0.27
DPI	Air mediated effects	0.00	0.21	0.14	0.06	0.09	0.00	0.20	0.02	0.20
PP	log (BCF*)	0.50	1.44	1.31	0.35	0.49	0.21	0.50	0.50	1.26
DPI	Accumulation	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PP	Substance type	organics								
DPI	Solid waste	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Safety		1.63	1.86	1.84	1.12	1.33	1.39	1.68	1.87	1.17
Health		0.93	1.21	1.16	0.72	0.76	0.79	1.01	1.17	0.80
Environment		0.79	1.06	0.86	0.87	0.88	0.77	1.20	1.17	0.90
EHS		3.35	4.13	3.86	2.70	2.96	2.95	3.89	4.21	2.87

\*BCF: Bioconcentration factor

**Table C2(a):** LCA metrics as predicted by the FineChem<sup>23</sup> tool for the solvents of Figure 4a. MEA is also included for reference and 4AP data can be found in Table C1a.

LCA metrics	MEA	2AP	MMEA	EMEA	MPA	DEAB	2A1B	2A1PN	IPAE	DBA
CED (MJ-eq/kg)	105.5	105.8	105.8	106.1	105.8	108.7	106.1	106.7	106.7	93.5
GWP (kg CO <sub>2</sub> -eq/kg)	3.5	3.4	3.4	3.4	3.4	3.2	3.4	3.4	3.4	3.6
EI-99 (pt/kg)	0.18	0.20	0.20	0.22	0.20	0.25	0.22	0.22	0.23	0.30

**Table C2(b):** EHS index values and their decomposition into safety, health and environment categories, dangerous properties (index) and related indicators for the solvents of Figure 4a (e.g., the indicator “boiling point” is used to derive the value of the dangerous property called “mobility”). MEA is also included for reference and 4AP data can be found in Table C1b.

	Primary and Dangerous properties	MEA	2AP	MMEA	EMEA	MPA	DEAB	2A1B	2A1PN	IPAE	DBA
PP	Boiling point ( °C)	129	134	126	151	153	208	158	180	165	165
DPI	Mobility	0.58	0.55	0.59	0.49	0.48	0.26	0.46	0.37	0.43	0.43
PP	Flashpoint ( °C)	85	71	76	71	79	72	82	95	70	40
DPI	Flammability	0.84	0.87	0.87	0.85	0.83	0.80	0.82	0.77	0.84	0.92
PP	LD50oral (mg/kg)	(30pp m)	1765	R-phrase (R21/22)	EU-c(T)	R-phrase (R20/21/ 22)	1659	1989	4351	1968	EU-c (Xn)
DPI	Acute toxicity	0.79	0.20	0.36	0.56	0.31	0.00	0.09	0.00	0.07	0.29
PP	Oxygen balance (%)	-170.3	-202.4	-202.4	-224.4	-202.4	-269.9	-224.4	-240.4	-240.4	-315.7
DPI	Reaction/ Decomposition	0.00	0.00	0.00	0.00	0.00	0.00	0.14	0.00	0.00	0.15
PP	LD50 <sub>dermal</sub> (mg/kg)	EU-c (C)	EU-c (C)	EU-c (C)	R-code (R34)	EU-c (C)	PH (12.52)	PH (12.05)	PH (12.05)	PH (12.12)	768
DPI	Irritation	0.87	0.86	0.87	0.84	0.84	0.82	0.81	0.77	0.82	0.39
PP	Acute toxicity	0.79	0.20	0.36	0.56	0.31	0.00	0.09	0.00	0.07	0.29
DPI	Chronic toxicity	0.64	0.08	0.29	0.44	0.08	0.00	0.04	0.00	0.02	0.21
PP	Persistency (days)	25	24	24	25	25	22	25	25	24	11
DPI	Environmental Degradation	0.69	0.69	0.69	0.69	0.70	0.67	0.70	0.70	0.69	0.52
PP	LC50aq(mg/l)	502	267	331	294	543	119	116	73	277	49
DPI	Water mediated effects	0.04	0.07	0.06	0.07	0.03	0.15	0.16	0.21	0.07	0.20
PP	Chronic toxicity	0.64	0.08	0.29	0.44	0.08	0.00	0.04	0.00	0.02	0.21
DPI	Air mediated effects	0.58	0.03	0.22	0.42	0.07	0.05	0.05	0.00	0.04	0.18
PP	log (BCF)	0.50	0.50	0.50	0.50	0.50	0.45	0.50	0.09	0.12	1.53
DPI	Accumulation	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PP	Substance type	organic	organic	organic	organic	organic	organic	organic	organic	organic	organic
DPI	Solid waste	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Safety		2.20	1.63	1.82	1.90	1.62	1.05	1.51	1.14	1.35	1.79
Health		1.51	0.94	1.16	1.28	0.92	0.82	0.86	0.77	0.84	0.60
Environment		1.31	0.79	0.97	1.18	0.80	0.86	0.90	0.91	0.80	0.90
EHS		5.02	3.36	3.95	4.37	3.34	2.74	3.26	2.82	2.98	3.28

\*BCF: Bioconcentration factor

**Table C3(a):** LCA metrics as predicted by the FineChem<sup>23</sup> tool for the design solvents of Figure 5. The absence of data for E7 and D6 is elaborated in the caption of Figure 5.

LCA metrics	D1	D2	D3	D4	D5	D7	D8	D9	D10
CED (MJ-eq/kg)	164.6	150.5	148.9	149.0	148.8	140.6	175.3	176.6	180.4
GWP (kg CO <sub>2</sub> -eq/kg)	6.9	4.2	5.8	6.0	5.7	4.2	6.9	6.8	7.1
EI-99 (pt/kg)	1.05	0.59	0.98	1.00	0.98	0.51	0.36	0.41	0.46

**Table C3(b):** EHS index values and their decomposition into safety, health and environment categories, dangerous properties (index) and related indicators for the solvents of Figure 5 (e.g., the indicator “boiling point” is used to derive the value of the dangerous property called “mobility”). The absence of data for E7 and D6 is elaborated in the caption of Figure 5.

	Primary and Dangerous properties	D1	D2	D3	D4	D5	D7	D8	D9	D10
PP	Boiling point (°C)	222	197	195	225	195	203	184	206	203
DPI	Mobility	0.20	0.30	0.31	0.19	0.31	0.28	0.35	0.27	0.28
PP	Flashpoint (°C)	90	67	68	118	90	83	84	100	89
DPI	Flammability	0.74	0.82	0.82	0.66	0.76	0.77	0.79	0.73	0.76
PP	LD50oral (mg/kg)	584	761	849	1114	1066	1232	2301	1986	1879
DPI	Acute toxicity	0.00	0.05	0.05	0.00	0.02	0.00	0.00	0.00	0.00
PP	Oxygen balance (%)	-266.20	-262.15	-258.86	-266.20	-249.95	-262.15	-	-216.61	-216.61
DPI	Reaction/ Decomposition	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.20	0.20
PP	PH	12.06	12.08	11.68	12.07	11.61	12.17	11.42	11.63	11.62
DPI	Irritation	0.69	0.74	0.65	0.68	0.63	0.75	0.60	0.61	0.61
PP	Acute toxicity	0.00	0.05	0.05	0.00	0.02	0.00	0.00	0.00	0.00
DPI	Chronic toxicity	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PP	Persistency (days)	64	44	51	62	28	31	24	25	25
DPI	Environmental Degradation	0.90	0.82	0.85	0.90	0.72	0.74	0.69	0.69	0.70
PP	LC50aq(mg/l) Water	5	67	28	7	19	47	26	185	27
DPI	mediated effects	0.55	0.25	0.35	0.51	0.36	0.26	0.32	0.10	0.32
PP	Chronic toxicity	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DPI	Air mediated effects	0.26	0.20	0.20	0.20	0.12	0.11	0.03	0.04	0.05
PP	log (BCF)	0.28	0.41	0.13	0.26	-0.02	0.37	-0.01	-0.07	-0.01
DPI	Accumulation	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PP	Substance type	organics								
DPI	Solid waste	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Safety		0.94	1.17	1.18	0.85	1.09	1.05	1.14	1.19	1.23
Health		0.69	0.74	0.65	0.68	0.63	0.75	0.60	0.61	0.61
Environment		1.71	1.26	1.41	1.60	1.20	1.12	1.04	0.84	1.06
EHS		3.33	3.17	3.23	3.14	2.92	2.92	2.79	2.65	2.91

\*BCF: Bioconcentration factor

**Table C4:** Data sources for the primary properties used in the EHS assessment. MSDS stands for Material and Safety Data Sheets

Primary Property	Source
Boiling point	Marrero and Gani <sup>20</sup>
Flash point	MSDS, the US EPA's Toxicity Estimation Software Tool (TEST) V4.1 <sup>96</sup>
LD50 <sub>oral</sub>	MSDS, TEST, Discovery Studio V3.5 <sup>31</sup>
Oxygen balance	Chetah V9.0 <sup>144</sup>
LD50 <sub>dermal</sub>	MSDS
LC50 aquatic	Ecological Structure Activity Relationships (ECOSAR) Class Program V1.0, part of the US EPA's Estimation Program Interface (EPI) Suite <sup>TM</sup> V4.1 <sup>30</sup>
Persistence	Level III Fugacity model EPI Suite V4.1 <sup>30</sup>
Bio-concentration factor (BCF)	EPI Suite V4.1 <sup>30</sup>
pKa	Marvin 6.0.5 <sup>22</sup>
IDLH	MSDS
Risk phrases	MSDS
EU Classification	MSDS

#### Section D: The SAFT- $\gamma$ SW model

The SAFT- $\gamma$  SW<sup>32, 33</sup> equation of state is used in Stage 2 to evaluate solvent performance. It is a molecular-based equation of state where molecules are modelled as chains of fused heteronuclear segments interacting via a variable range potential (here, a square-well potential). Each segment, or group of segments, represents a different chemical moiety or functional group in the molecule. Association sites are added where appropriate to mediate hydrogen-bonding interactions or even chemical aggregation of species<sup>34, 35</sup>. The SAFT- $\gamma$  SW formalism is a generalisation of the SAFT-VR homonuclear approach<sup>36, 37</sup> which has been shown to provide an accurate description of the thermodynamic fluid-phase behaviour of a wide variety of compounds and their mixtures, including mixtures of CO<sub>2</sub>, water and amines<sup>34, 38, 39</sup>. The reformulation of the SAFT-VR EoS within a GC framework, in the form of the SAFT- $\gamma$  SW EoS, increases the predictive capability of the approach significantly. This is due to the underlying assumption (as in any GC approach) that once the parameters for a particular functional group have been determined from regression to experimental data for specific molecules, they can be transferred to other molecules that contain this functional group without any further parameter adjustment. This can be used to predict the fluid-phase behaviour of compounds whose properties have not yet been measured experimentally.

A first step towards the description of multifunctional amines, and their mixtures with water and CO<sub>2</sub>, with the SAFT- $\gamma$  SW EoS was presented in Chremos et al.<sup>40</sup>. It has been extended in subsequent studies<sup>41, 42</sup>. Several strategies have been developed in this previous work to tackle the challenges associated with modelling these complex mixtures in a predictive way. Multifunctional compounds such as alkanolamines present highly polarisable functional groups (e.g., hydroxyl and amine) that can be in close proximity; this can alter the effective interactions of these groups with other molecules. Specialised (higher-order) groups have been developed to account for such proximity effects<sup>40-42</sup>. The reactive nature of the mixtures is modelled implicitly, using strong physical interactions between association sites to mimic the formation of

new species<sup>34, 38, 39, 40-42</sup>. In our current work, we use the SAFT- $\gamma$  SW EoS and the parameters developed in previous works<sup>40-43</sup> to describe aqueous mixtures of selected multifunctional amines with carbon dioxide.

Within SAFT- $\gamma$  SW molecules are modelled as heteronuclear chains, where each segment characterises a given chemical moiety. Dispersion interactions between segments are described via square-well potentials and association sites are used to mimic strong directional interactions such as hydrogen bonds. A given functional group  $k$  is characterised by the number  $v_k^*$  of identical segments it comprises, the hard-core diameter  $\sigma_{kk}$  of each segment, the depth  $\varepsilon_{kk}$  and range  $\lambda_{kk}$  of the segment-segment dispersion interactions, the depth  $\varepsilon^{\text{HB}}_{kkab}$  and the range  $r_{c,kkab}$  of the hydrogen-bonding interactions between association site types  $a$  and  $b$ , and the shape factor  $S_k$  or the degree to which the given functional group contributes to the overall properties of the molecule. The molecular model parameters characterising each functional group have been developed in previous works<sup>40, 41, 43</sup>. In Tables D1, D2 and D3 we summarise the ones used in this work for completeness.

**Table D1:** SAFT- $\gamma$  SW like group parameters (see text for details).  $N_{k,e}$ ,  $N_{k,H}$ ,  $N_{k,\alpha 1}$  and  $N_{k,\alpha 2}$  represent the number of association sites of type e, H,  $\alpha_1$  and  $\alpha_2$ , respectively, on group  $k$ .  $k_B$  is Boltzmann's constant.

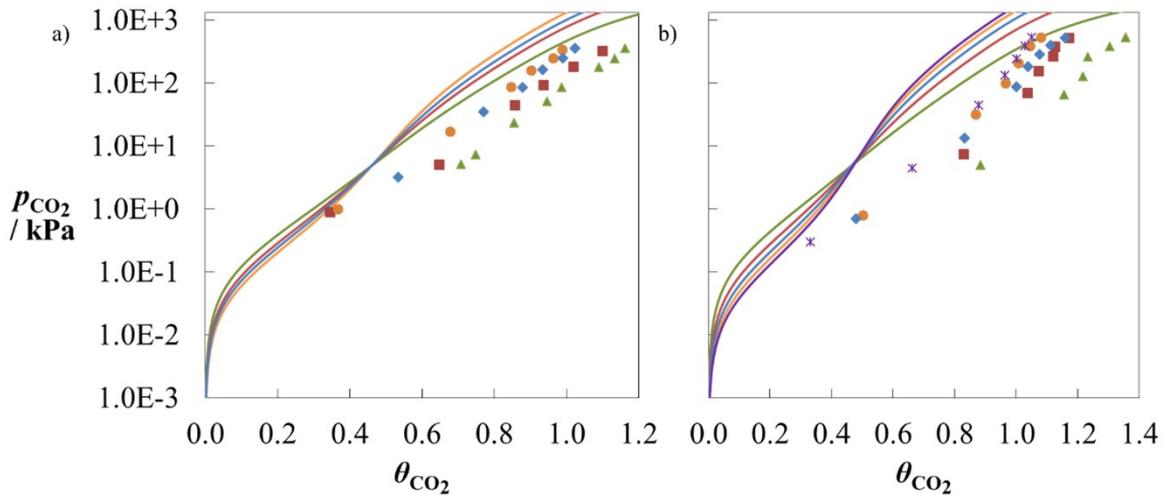
Group	$v_k^*$	$S_k$	$\sigma_{kk} / \text{\AA}$	$\lambda_{kk}$	$(\varepsilon_{kk}/k_B) / \text{K}$	$(\varepsilon_{kkab}/k_B) / \text{K}$	$r_{c,kkab} / \text{\AA}$	$N_{k,e}$	$N_{k,H}$	$N_{k,\alpha 1}$	$N_{k,\alpha 2}$
CH <sub>3</sub>	1	0.6667	3.8105	1.4130	252.601	-	-	-	-	-	-
CH <sub>2</sub>	1	0.3333	4.0276	1.6606	240.482	-	-	-	-	-	-
CH <sub>2</sub> NH <sub>2</sub>	1	0.9075	3.8080	1.4836	439.350	1021.375	2.4450	1	2	-	-
CH <sub>2</sub> NH	1	0.3600	4.8000	1.6200	173.605	990.075	2.8302	1	1	-	-
CH <sub>2</sub> OH	1	0.5657	4.3174	1.6519	399.959	2555.721	2.3598	2	1	-	-
CHOH	1	0.8998	3.5251	1.2823	575.000	1522.668	2.3362	2	1	-	-
H <sub>2</sub> O	1	1.0000	3.0342	1.7889	250.000	1400.000	2.1082	2	2	-	-
CO <sub>2</sub>	2	1.0000	2.7865	1.5157	179.270	-	-	-	-	1	1

**Table D2:** SAFT- $\gamma$  SW unlike group dispersion interaction energies  $\varepsilon_{kl}$ . The numbers in brackets correspond to the unlike values of the range  $\lambda_{kl}$ ; in all other cases the combining rule  $\lambda_{ij} = (\lambda_{ii}\sigma_{ii} + \lambda_{jj}\sigma_{jj})/(\sigma_{ii} + \sigma_{jj})$ , is used. The table is symmetric ( $\varepsilon_{kl} = \varepsilon_{lk}$ ). The group CH<sub>2</sub>NH<sub>2</sub>[CH<sub>2</sub>OH] refers to a CH<sub>2</sub>NH<sub>2</sub> affected by the presence of a CH<sub>2</sub>OH group bonded to it.

Group	CH <sub>3</sub>	CH <sub>2</sub>	CH <sub>2</sub> NH <sub>2</sub>	CH <sub>2</sub> NH <sub>2</sub> [CH <sub>2</sub> OH]	CH <sub>2</sub> NH	CH <sub>2</sub> OH	CHOH	H <sub>2</sub> O
CH <sub>3</sub>	-	-	-	-	-	-	-	-
CH <sub>2</sub>	261.520	-	-	-	-	-	-	-
CH <sub>2</sub> NH <sub>2</sub>	254.736	297.873	-	-	-	-	-	-
CH <sub>2</sub> NH	374.600	275.940	108.707	-	-	-	-	-
CH <sub>2</sub> OH	279.939	283.702	143.247	143.247	110.247	-	-	-
CHOH	465.942	367.465	365.774	-	138.101	-	-	-
H <sub>2</sub> O	460.312	460.276	286.857	444.924	369.506	328.263	399.643	-
	(1.257)	(1.257)	(1.740)	(1.279)	(1.800)			
CO <sub>2</sub>	196.296	189.721	480.501	383.850	200.000	245.442	318.628	224.400
			(1.293)	(1.293)	(1.293)			

**Table D3:** SAFT- $\gamma$  SW association energies and ranges between the different site types in different groups. The group  $\text{CH}_2\text{NH}_2[\text{CH}_2\text{OH}]$  refers to a  $\text{CH}_2\text{NH}_2$  affected by the presence of a  $\text{CH}_2\text{OH}$  group bonded to it.

Group (site type)	$\text{CH}_2\text{NH}_2$ (e)	$\text{CH}_2\text{NH}_2$ (H)	$\text{CH}_2\text{NH}_2$ [ $\text{CH}_2\text{OH}$ ] (e)	$\text{CH}_2\text{NH}_2$ [ $\text{CH}_2\text{OH}$ ] (H)	$\text{CH}_2\text{NH}$ (e)	$\text{CH}_2\text{NH}$ (H)	$\text{CH}_2\text{OH}$ (e)	$\text{CH}_2\text{OH}$ (H)	$\text{CHOH}$ (e)	$\text{CHOH}$ (H)
$\text{CH}_2\text{OH}$ (e)	-	1696.979 (2.5282)	-	1696.979 (2.5282)	-	1883.891 (3.4281)	-	-	-	-
$\text{CH}_2\text{OH}$ (H)	903.303 (3.9520)	-	903.303 (3.9520)	-	1471.500 (2.9028)	-	-	-	-	-
$\text{CH}_2\text{NH}$ (e)	-	-	-	-	-	-	-	1471.500 (2.9028)	-	808.014 (3.3209)
$\text{CH}_2\text{NH}$ (H)	-	-	-	-	-	-	1883.891 (3.4281)	-	750.256 (3.3151)	-
$\text{H}_2\text{O}$ (e)	-	1365.326 (2.3082)	-	1365.326 (2.3082)	-	1500.178 (2.4300)	-	1905.280 (2.4669)	-	1040.175 (2.4500)
$\text{H}_2\text{O}$ (H)	1261.968 (2.5200)	-	1261.968 (2.5200)	-	1380.930 (2.4100)	-	2122.971 (2.0186)	-	1070.150 (2.5500)	-
$\text{CO}_2(\alpha_1)$	4175.000 (1.9699)	-	4875.734 (1.9699)	-	3375.000 (2.2199)	-	-	-	-	-
$\text{CO}_2(\alpha_2)$	4870.194 (1.9790)	-	5175.024 (1.9790)	-	4475.000 (2.2500)	-	-	-	-	-



**Figure D1:** Solubility of  $\text{CO}_2$  in aqueous solutions of (a) MMEA and (b) EMEA at 303.1 K represented as mole fraction of  $\text{CO}_2$  as a function of the partial pressure along the vapour-liquid equilibrium of the ternary mixture (a) MMEA +  $\text{H}_2\text{O}$  +  $\text{CO}_2$  or (b) EMEA +  $\text{H}_2\text{O}$  +  $\text{CO}_2$ . The solubility is represented as  $\text{CO}_2$  loading  $\theta_{\text{CO}_2}$ , defined as the moles of  $\text{CO}_2$  absorbed in the liquid phase per mole of amine in the liquid. The symbols correspond to (a) experimental data<sup>44, 45</sup> for aqueous solutions of MMEA of various weight percentages in mass: 6.8 wt% (green), 11 wt% (red), 14 wt% (blue) and 19 wt% (orange), and to (b) experimental data<sup>46</sup> for aqueous solutions of EMEA of various weight percentages in mass: 6 wt% (green), 12 wt% (red), 18 wt% (blue) and 24 wt% (orange) and 30 wt% (purple). The solid curves correspond to SAFT- $\gamma$  SW calculations for the same percentages.

## Section E: Data for reported solvents

**Table E1:** Names, abbreviations, CAS numbers and literature sources of the amines contained in the Reference (R) class.

ID	Name	Abbrev.	CAS Registry Number	Source
R1	2-(Amino)-propanol	2AP	6168-72-5	Da Silva <sup>47</sup>
R2	2-Amino-2-methyl-1-propanol	AMP	124-68-5	Harbou et al. <sup>48</sup>
R3	2-(Methylamino)-ethanol	MMEA	109-83-1	Ma'mun et al. <sup>49</sup>
R4	Ethylaminoethanol	EMEA	110-73-6	Kumar et al. <sup>50</sup>
R5	2-(Butylamino) ethanol	BEA	111-75-1	Yamada et al. <sup>2</sup>
R6	N,N-Dimethylaminoethanol	DMMEA	108-01-0	Tong <sup>51</sup>
R7	N,N-Diethyl-2-aminoethanol	DEEA	100-37-8	Sutar et al. <sup>52</sup>
R8	3-Amino-1-propanol	MPA	156-87-6	Henni et al. <sup>53</sup>
R9	4-Diethylamino-2-butanol	DEAB	5467-48-1	Sema et al. <sup>54</sup>
R10	N-(2-aminoethyl) ethanolamine	AAEA	111-41-1	Stec et al. <sup>55</sup>
R11	Diethanolamine	DEA	111-42-2	Oexmann <sup>56</sup>
R12	Diethylenetriamine	DETA	111-40-0	Kim and Svendsen <sup>57</sup>
R13	Diisopropanolamine	DIPO	110-97-4	Oexmann <sup>56</sup>
R14	Ethylenediamine	EDA	107-15-3	Bishnoi <sup>58</sup>
R15	N-Methyl-1,3-propanediamine	MAPA	6291-84-5	Kim and Svendsen <sup>57</sup>
R16	Methyldiethanolamine	MDEA	105-59-9	Kim and Svendsen <sup>57</sup>
R17	Monoethanolamine	MEA	141-43-5	Oexmann <sup>56</sup>
R18	1,2-Propanediamine	MEDA	78-90-0	Rochelle <sup>59</sup>
R19	Tetraethylenepentamine	TEPA	112-57-2	Aronu et al. <sup>60</sup>
R20	Triethanolamine	TEA	102-71-6	Vertseeg et al. <sup>61</sup>
R21	Triisopropanolamine	TIPA	122-20-3	Chahuan et al. <sup>62</sup>
R22	Tromethamine	TRIS	77-86-1	Penders et al. <sup>63</sup>
R23	2-Amino-2-methyl-1,3-propanediol	AMPD	115-69-5	Penders et al. <sup>63</sup>
R24	2-Amino-2-ethyl-1,3-propanediol	AEPD	115-70-8	Baek and Yoon <sup>64</sup>
R25	3-(Dimethylamino)-1,2-propanediol	DMAPD	623-57-4	Lijima and Mitsuoka <sup>65</sup>

**Table E2:** Names, abbreviations, CAS numbers and literature sources of the amines selected from the Commercial (C) class. The amines were obtained from an in-house data repository at ETH Zurich, publicly available databases<sup>67, 67</sup> and the commercial catalogue of Sigma-Aldrich<sup>68</sup>.

ID	Name	Abbrev.	CAS Registry Number	Source
C1	2-Amino-1-butanol	2A1B	96-20-8	Rooney <sup>69</sup>
C2	2-Amino-1-pentanol	2A1PN	4146-04-7	Rooney <sup>69</sup>
C3	2-Amino-1-hexanol	2A1H	5665-74-7	Rooney <sup>69</sup>
C4	2-Propylamino-ethanol	PAE	16369-21-4	Yamada et al. <sup>70</sup>
C5	1-Methylamino-propan-2-ol	1M2P	16667-45-1	-
C6	2-(Isopropylamino)-ethanol	IPAE	109-56-8	Yamada et al. <sup>70</sup>
C7	Diisobutylamine	DIBA	626-23-3	Zhang et al. <sup>71, 72</sup>
C8	Di-sec butylamine	DsBA	110-96-3	Zhang et al. <sup>71, 72</sup>
C9	Di-N-Propylethylamine	DPE	20634-92-8	-
C10	4-Amino-2-butanol	4A2B	39884-48-5	-
C11	Di-N-butylamine	DBA	111-92-2	Zhang et al. <sup>71</sup>
C12	3-(Diethyl-amino)-propanol	3DAP	622-93-5	-
C13	N,N Diethyl-1-butanamine	ND1B	4444-68-2	-
C14	1-Ethyl-N,N-dimethylbutylamine	1EDB	24552-03-2	-
C15	N,N,N',N'-Tetramethyl-1,2-ethanediamine	TMEDA	110-18-9	Bouzina et al. <sup>73</sup>
C16	N,N,N',N',2-Pentamethyl-1,2-propanediamine	2P12P	68367-53-3	-
C17	4-Amino-pentanol	4AP	927-55-9	-
C18	5-Amino-penanol	5AP	2508-29-4	Singh et al. 6, 7, 74
C19	Hexanamine	HEXA	111-26-2	Zhang et al. <sup>71</sup> ; Singh et al. 6, 74
C20	4-(Dimethylamino)-1-butanol	4D1B	13330-96-6	-

**Table E3:** Names and CAS numbers amines C21-C60 in the Commercial (C) class. The amines were obtained from an in-house data repository at ETH Zurich, publicly available databases<sup>66, 67</sup> and the commercial catalogue of Sigma-Aldrich<sup>68</sup>.

ID	Name	CAS Registry Number	ID	Name	CAS Registry Number
C21	3-Methyl-3-(N-methyl-N-isopropyl)amin-2-butanol	64037-42-9	C41	2-Methylundecan-2-amine	110-10-1
C22	1-amino-2,2-dimethylpropan-1-ol	40898-98-4	C42	2-Methyl-6-methylamino-2-heptanol	17086-16-7
C23	N'-butyl-2-methyl-1,2-propanediamine	50540-24-4	C43	(2-Amino-2-methylpropyl)(propan-2-yl)amine	5448-29-3
C24	N-(3-hydroxypropyl)-1,2-propanediamine,	10171-78-5	C44	N-Methyl-N,1,1-triethyl-propylamine	33326-98-6
C25	2,2-dimethyl-1,3-propanediamine,	7328-91-8	C45	2-[(Octan-2-yl)amino]ethan-1-ol	26535-68-2
C26	1,3-Butanediamine	590-88-5	C46	1-(N,N-dimethyl)-1,2-Butanediamine	63732-18-3
C27	N,N,2,2-tetramethyl-1,3-propanediamine	53369-71-4	C47	Ethyl(methyl)(2,3,3-trimethylbutan-2-yl)amine	-
C28	Dimethyl(2,3,3-trimethylbutan-2-yl)amine	29773-01-1	C48	(3-Aminopropyl)(octyl)amine	7173-57-1
C29	N,N,N,N -tetramethyl-1,3-butanediamine	97-84-7	C49	2-[(3-Aminopropyl)(methyl)amino] ethan-1-ol	41999-70-6
C30	(3-Amino-2-methylpropyl)dimethylamine	6105-72-2	C50	(4-Aminobutyl)diethylamine	27431-62-5
C31	6-Amino-2-methyl-2-heptanol	372-66-7	C51	N,N,N'-triethyl-1,2-Ethanediamine	105-04-4
C32	4,5-Dimethylheptane-1,6-diamine	25620-58-0	C52	2-{[3-(Dimethylamino)propyl](2-methylpropyl)amino}ethan-1-ol	78718-56-6
C33	1-Amino-2-methylbutan-2-ol	51411-49-5	C53	(4-Methylpentan-2-yl)({2-[(4-methylpentan-2-yl)amino]ethyl})amine	-
C34	2,4-Dimethyl-3-pentanamine	4083-57-2	C54	2-[(4-aminopentyl)(ethyl)amino] ethan-1-ol	69559-11-1
C35	1-Amino-3-diethylamino-propan-2-ol	6322-06-1	C55	2-Undecanamine	13205-56-6
C36	Ethyl(3-methylpentan-3-yl)amine	1185-93-9	C56	N-(2-Aminoethyl)-N,N'-dimethyl-1,2-ethanediamine	-
C37	2-Amino-2-methyl-3-hexanol	63765-79-7	C57	N2,N2-dimethyl-1,2-propanediamine	19764-58-0
C38	2-{[3-(dimethylamino)-2,2-dimethylpropyl]amino}ethan-1-ol	84642-65-9	C58	1-(Decylamino)propan-2-ol	68603-41-8
C39	3,3-Dimethyl butylamine	15673-00-4	C59	N,N-diethyl-1-dodecanamine	4271-27-6
C40	(4-Aminopentyl)diethylamine	140-80-7	C60	2-[(1-Hydroxypropan-2-yl)(methyl)amino]propan-1-ol	56684-95-8

**Table E4:** Names and CAS numbers amines C61-C101 in the Commercial (C) class. The amines were obtained from an in-house data repository at ETH Zurich, publicly available databases<sup>66, 67</sup> and the commercial catalogue of Sigma-Aldrich<sup>68</sup>.

ID	Name	CAS Registry Number	ID	Name	CAS Registry Number
C61	1,1-Dimethyl-2-pentyl-hydrazine	67398-36-1	C82	N-octyl-1-octanamine	1120-48-5
C62	N-(1-methylethyl)-1-butanamine	39099-23-5	C83	N,N-dipentyl-1-pentanamine	621-77-2
C63	N,N-dipropyl-1-Propanamine	102-69-2	C84	N-methyl-N-(N,N-dimethylaminoethyl)-aminoethanol	2212-32-0
C64	N-methyl-1-octanamine	2439-54-5	C85	N,N-Diethyl-2-aminoethanol	100-37-8
C65	N,N-dimethyl-1,3-propanediamine	109-55-7	C86	1,3-bis(Dimethylamino)-2-propanol	5966-51-8
C66	1-Nonanamine	112-20-9	C87	1,8-Diaminooctane	373-44-4
C67	1-Octanamine	111-86-4	C88	1,7-Diaminoheptane	646-19-5
C68	1-Decanamine	2016-57-1	C89	1,6-Hexanediamine	124-09-4
C69	1-Heptanamine	111-68-2	C90	1,5-Pentanediamine	462-94-2
C70	N-pentyl-1-pentanamine	2050-92-2	C91	1,4-Butanediamine	110-60-1
C71	2-Dimethylamino-2-methylpropanol	7005-47-2	C92	1,3-Propanediamine	109-76-2
C72	1-Dodecanamine	124-22-1	C93	1-Amino-2-propanol	78-96-6
C73	2-Methyl-1,2-propanediamine	811-93-8	C94	5-Amino-2,2-dimethylpentanol	13532-77-9
C74	N-hexyl-1-Hexanamine	143-16-8	C95	6-Amino-1-hexanol	4048-33-3
C75	2-Amino-3-methyl-1-butanol	16369-05-4	C96	4-Amino-1-butanol	13325-10-5
C76	(Diisopropylamino)ethanol	96-80-0	C97	2-Amino-1,3-propanediol	534-03-2
C77	Tributylamine	102-82-9	C98	3-(Diethylamino)-1,2-propanediol	621-56-7
C78	N,N-dimethyl- 1-decanamine	1120-24-7	C99	Ethyldiethanolamine	139-87-7
C79	3-(Dimethylamino)-1-propanol	3179-63-3	C100	2,2'-(Butylimino)bis-ethanol,	102-79-4
C80	1-(Dimethylamino)-2-propanol	108-16-7	C101	3-Methylamino-1,2-propanediol	40137-22-2
C81	2-(tert-Butylamino)ethanol	4620-70-6	-	-	-

**Table E5:** Molecular structures obtained from CAMD in D class (D1-D78).

ID	Groups in molecule	Frequency of groups	ID	Groups in molecule	Frequency of groups
D1	$[-\text{CH}_3, >\text{CH}_2, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{NH}-, -\text{CH}_2-\text{N}<]$	[4 1 1 1 1]	D40	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{N}<]$	[1 2 2 1]
D2	$[-\text{CH}_3, >\text{CH}_2, >\text{C}<, -\text{OH}, ->\text{C}-\text{NH}_2]$	[4 1 1 1 1]	D41	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2]$	[1 1 1 2]
D3	$[-\text{CH}_3, >\text{CH}_2, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[3 1 1 1 1]	D42	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{NH}-]$	[2 1 1 1]
D4	$[-\text{CH}_3, >\text{CH}_2, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{NH}-]$	[3 2 1 2]	D43	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, >\text{CH}-\text{NH}-]$	[2 1 2 1]
D5	$[-\text{CH}_3, >\text{CH}_2, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{NH}-]$	[2 1 1 1 1]	D44	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, \text{CH}_3-\text{N}<, -\text{CH}_2-\text{N}<]$	[1 1 2 1 1]
D6	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{CH}_2-\text{NH}-, -\text{CH}_2-\text{N}<]$	[5 1 1 1 2]	D45	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[1 1 1 1 1]
D7	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, ->\text{C}-\text{NH}_2]$	[3 2 1 1 1]	D46	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[1 2 1 1 1]
D9	$[-\text{CH}_3, -\text{OH}, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{NH}-]$	[2 1 1 1]	D47	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[2 1 1 1 1]
D9	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[1 2 1 2]	D48	$[-\text{CH}_3, -\text{OH}, \text{CH}_3-\text{N}<, -\text{CH}_2-\text{N}<]$	[1 2 2 1]
D10	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{NH}-]$	[2 1 1 1 1]	D49	$[-\text{CH}_3, -\text{OH}, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[1 1 1 2]
D11	$[-\text{OH}, >\text{CH}-\text{NH}_2]$	[2 1]	D50	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{N}<]$	[2 1 1 1 1]
D12	$[-\text{OH}, -\text{CH}_2-\text{NH}-]$	[2 1]	D51	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-, -\text{CH}_2-\text{N}<]$	[1 1 2 1 1]
D13	$[-\text{CH}_3, -\text{OH}, ->\text{C}-\text{NH}_2]$	[1 2 1]	D52	$[-\text{CH}_3, >\text{CH}_2, >\text{C}<, -\text{OH}, \text{CH}_3-\text{N}<]$	[2 1 1 2 1]
D14	$[>\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2]$	[1 2 1]	D53	$[-\text{CH}_3, >\text{CH}_2, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[1 1 1 2]
D15	$[-\text{OH}, \text{CH}_3-\text{N}<]$	[2 2]	D54	$[-\text{CH}_3, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{N}<]$	[2 1 1 2]
D16	$[>\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[1 2 1]	D55	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{N}<]$	[1 2 1 2 1]
D17	$[-\text{OH}, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[2 1 1]	D56	$[-\text{CH}_3, -\text{OH}, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[1 1 2 1]
D18	$[-\text{CH}_3, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[1 1 1 1]	D57	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[1 2 1 2 1]
D19	$[>\text{CH}_2, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{NH}-]$	[1 1 2 1]	D58	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[2 2 2 1]
D20	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{N}<]$	[2 2 1]	D59	$[-\text{CH}_3, -\text{OH}, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{N}<]$	[3 1 1 1]
D21	$[>\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2]$	[2 2 1]	D60	$[>\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[3 1 1 1]
D22	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{N}<]$	[1 1 2 1]	D61	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, -\text{CH}_2-\text{N}<]$	[2 1 1 2 1]
D23	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, >\text{CH}-\text{NH}_2]$	[1 1 2 1]	D62	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{NH}-]$	[3 1 1 1]
D24	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{N}<]$	[1 2 2]	D63	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2, \text{CH}_3-\text{N}<]$	[1 1 1 1 2]
D25	$[>\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[2 2 1]	D64	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, \text{CH}_3-\text{N}<, -\text{CH}_2-\text{N}<]$	[1 2 2 1 1]
D26	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[1 1 2 1]	D65	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{N}<, -\text{CH}_2-\text{N}<]$	[2 1 2 1 1]
D27	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}-]$	[1 1 2 1]	D66	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2, -\text{CH}_2-\text{NH}-]$	[1 2 1 1 1]
D28	$[-\text{CH}_3, -\text{OH}, \text{CH}_3-\text{N}<, -\text{CH}_2-\text{N}<]$	[1 2 1 1]	D67	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[1 1 1 1 1 1]
D29	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[1 1 1 1 1]	D68	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{N}<]$	[2 1 2 1]
D30	$[-\text{CH}_3, -\text{OH}, -\text{CH}_2-\text{NH}-, -\text{CH}_2-\text{N}<]$	[1 2 1 1]	D69	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[1 1 1 1 2]
D31	$[>\text{CH}_2, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{NH}-]$	[2 1 2 1]	D70	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{N}<]$	[2 2 1 1 1]
D32	$[-\text{CH}_3, >\text{C}<, -\text{OH}, \text{CH}_3-\text{N}<]$	[2 1 2 1]	D71	$[-\text{CH}_3, >\text{CH}_2, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[1 2 1 2]
D33	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{N}<]$	[1 1 1 2 1]	D72	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{N}<]$	[2 1 1 1 2]
D34	$[>\text{CH}_2, -\text{OH}, \text{CH}_3-\text{N}<]$	[2 2 2]	D73	$[-\text{CH}_3, >\text{CH}-, ->\text{C}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[2 1 1 2]
D35	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{N}<]$	[1 1 2 2]	D74	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, \text{CH}_3-\text{N}<]$	[2 1 2 2 1]
D36	$[>\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[3 2 1]	D75	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{N}<]$	[2 1 2 2]
D37	$[-\text{CH}_3, >\text{CH}_2, >\text{CH}-, -\text{OH}, -\text{CH}_2-\text{NH}-]$	[1 1 1 2 1]	D76	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}-, \text{CH}_3-\text{N}<]$	[1 1 1 2 1]
D38	$[>\text{CH}_2, -\text{OH}, >\text{CH}-\text{NH}_2, \text{CH}_3-\text{NH}-]$	[2 1 1 1]	D77	$[-\text{CH}_3, >\text{CH}-, -\text{OH}, ->\text{C}-\text{NH}_2, -\text{CH}_2-\text{NH}-]$	[3 1 1 1 1]
D39	$[>\text{CH}_2, -\text{OH}, -\text{CH}_2-\text{NH}_2, \text{CH}_3-\text{N}<]$	[1 1 1 2]	D78	$[-\text{CH}_3, >\text{CH}_2, -\text{OH}, \text{CH}_3-\text{NH}-, -\text{CH}_2-\text{NH}-, -\text{CH}_2-\text{N}<]$	[1 1 1 1 1 1]

**Table E6:** Molecular structures obtained from CAMD in D class (D79-D157).

ID	Groups in molecule	Frequency of groups	ID	Groups in molecule	Frequency of groups
D79	[>CH <sub>2</sub> ,>CH-,-OH,CH <sub>3</sub> -NH-]	[3 1 1 2]	D119	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[3 1 1 2]
D80	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,-CH <sub>2</sub> -NH-]	[2 1 2 2 1]	D120	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,>C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[2 4 1 1 1]
D81	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[3 1 1 1 1]	D121	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 2 1 1 1 1]
D82	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-,CH <sub>3</sub> -N<]	[2 1 1 2]	D122	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,-CH <sub>2</sub> -NH-]	[1 4 1 2]
D83	[-CH <sub>3</sub> ,-OH,>CH-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-,CH <sub>2</sub> -N<]	[2 1 1 1 1]	D123	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,-CH <sub>2</sub> -NH-]	[2 2 1 1 2]
D84	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,>CH-NH <sub>2</sub> ,CH <sub>3</sub> -NH-]	[1 2 1 1 1 1]	D124	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-,CH <sub>2</sub> -NH-,CH <sub>2</sub> -N<]	[3 1 1 1 1]
D85	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C<,-OH,-CH <sub>2</sub> -N<]	[3 1 1 2 1]	D125	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,->C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-]	[2 2 1 1 2]
D86	[>CH <sub>2</sub> ,-OH,CH <sub>3</sub> -NH-,CH <sub>3</sub> -N<]	[3 1 1 2]	D126	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 2 1 1 1]
D87	[-CH <sub>3</sub> ,-OH,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[3 1 1 1 1]	D127	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[3 3 1 1 1]
D88	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,-CH <sub>2</sub> -N<]	[2 2 1 2 1]	D128	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-,CH <sub>3</sub> -N<]	[2 2 1 1 2]
D89	[-CH <sub>3</sub> ,-OH,-CH <sub>2</sub> -NH-,CH <sub>2</sub> -N<]	[2 1 2 1]	D129	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[4 1 1 1 1 1]
D90	[>CH <sub>2</sub> ,-OH,CH <sub>3</sub> -NH-,CH <sub>2</sub> -NH-]	[4 1 1 1]	D130	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 1 1 3]
D91	[-CH <sub>3</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[3 1 1 1]	D131	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[3 2 1 1 1 1]
D92	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,CH <sub>3</sub> -NH-,CH <sub>2</sub> -NH-]	[1 2 1 1 1 1]	D132	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-,CH <sub>3</sub> -N<]	[3 2 1 1 1]
D93	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,CH <sub>3</sub> -N<]	[1 2 1 3]	D133	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,-CH <sub>2</sub> -NH-,CH <sub>2</sub> -N<]	[2 2 1 2 1]
D94	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-,CH <sub>2</sub> -N<]	[2 1 2 1]	D134	[-CH <sub>3</sub> ,>CH-,-OH,-CH <sub>2</sub> -NH-,CH <sub>2</sub> -N<]	[3 1 1 2 1]
D95	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[2 1 1 2 1 1]	D135	[-CH <sub>3</sub> ,>CH-,-CH <sub>2</sub> -NH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[4 1 1 1 1]
D96	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,>CH-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[1 3 1 1 1]	D136	[-CH <sub>3</sub> ,-CH <sub>2</sub> -NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[2 2 3]
D97	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,>CH-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[2 1 1 1 1 1]	D137	[-CH <sub>3</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[4 1 1 1 1]
D98	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[3 1 2 ]	D138	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[4 1 1 1 2]
D99	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[2 3 1 1 1]	D139	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,-CH <sub>2</sub> -NH-]	[2 3 1 1 2]
D100	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,-CH <sub>2</sub> -NH-]	[1 3 1 2]	D140	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 3 1 2]
D101	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,-OH,-CH <sub>2</sub> -NH-]	[2 1 1 1 2]	D141	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 3 1 1 1]
D102	[-CH <sub>3</sub> ,>CH-,-OH,-CH <sub>2</sub> -NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[2 1 1 2 1]	D142	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[4 1 2 1]
D103	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-CH <sub>2</sub> -NH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[2 2 1 1 1]	D143	[-CH <sub>3</sub> ,>C<,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[5 1 1 1 1]
D104	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-,CH <sub>3</sub> -N<]	[2 2 1 1 1]	D144	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 3 1 1 1]
D105	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,CH <sub>3</sub> -NH-,CH <sub>2</sub> -NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[1 2 1 1 1 1]	D145	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 2 1 1 2]
D106	[>CH <sub>2</sub> ,>CH-,-OH,CH <sub>3</sub> -NH-]	[4 1 1 2]	D146	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[4 2 1 1 1]
D107	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,-CH <sub>2</sub> -NH <sub>2</sub> ,>CH-NH <sub>2</sub> -]	[2 2 1 1 1]	D147	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[4 2 1 1 1]
D108	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[2 1 2 1 2]	D148	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[3 3 1 2]
D109	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[3 1 1 1 1]	D149	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-]	[4 1 1 1 2]
D110	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>C<,-OH,-CH <sub>2</sub> -N<]	[3 2 1 2 1]	D150	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[4 1 1 1 1 1]

**Table E6** (Continued)

D111	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[3 1 1 1 1]	D151	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-, -CH <sub>2</sub> -N<]	[4 2 1 1 1]
D112	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,-OH,-CH <sub>2</sub> -NH-, -CH <sub>2</sub> -N<]	[2 1 1 2 1]	D152	[-CH <sub>3</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[5 1 1 2]
D113	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-NH <sub>2</sub> ,->C-NH <sub>2</sub> , -CH <sub>2</sub> -NH-]	[3 1 1 1 1]	D153	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-, CH <sub>3</sub> -N<]	[3 4 1 1 1]
D114	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -NH-, -CH <sub>2</sub> -N<]	[3 1 1 1 1]	D154	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,->C-NH <sub>2</sub> , -CH <sub>2</sub> -NH-,CH <sub>3</sub> -N<]	[4 1 1 1 1 2]
D115	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-,CH <sub>3</sub> -N<]	[3 1 1 2]	D155	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[4 3 1 1 1]
D116	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,CH <sub>3</sub> -N<]	[4 1 2 1]	D156	[-CH <sub>3</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -N<]	[6 2 2]
D117	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,>OH,>CH-NH <sub>2</sub> , -CH <sub>2</sub> -NH-]	[2 2 1 1 1 1]	D157	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,->C-NH <sub>2</sub> ,-CH <sub>2</sub> -NH-, CH <sub>3</sub> -N<,-CH <sub>2</sub> -N<]	[4 2 1 1 1 1]
D118	[-CH <sub>3</sub> ,>CH <sub>2</sub> ,>CH-,>OH,>C-NH <sub>2</sub> ]	[4 1 2 1 1]			

**Table E7:** Names, abbreviations, CAS numbers and literature sources of amines reported in the manuscript without being part of any of the investigated datasets.

ID	Name	Abbrev.	CAS Registry Number	Source
E1	Butylmonoethanolamine	BMEA	111-75-1	Rooney <sup>69</sup>
E2	1-Amino-2-propanol	MIPA	2799-16-8	Hamborg <sup>75</sup>
E3	Diisopropylamine	DIPA	142-84-7	Zhang et al. <sup>71</sup>
E4	Tributylamine	TBA	102-82-9	Zhang et al. <sup>71</sup>
E5	3-Dimethyl-amino-1-propanol	3DMA1P	3179-63-3	Kadiwala et al. <sup>76</sup>
E6	N,N-Dimethyl cyclohexylamine	DMCA	98-94-2	Zhang et al. <sup>71</sup>
E7	Bis-(3-dimethylaminopropanol)	TMBPA	6711-48-4	Aronu et al. <sup>4</sup>

### Section F: Assessment of the 29 solvents selected from the databases (Classes C and R)

The 29 solvents selected in Stage 1 for the Selection problem (Tables 4-6) are discussed here in terms of their structural characteristics and likely CO<sub>2</sub> capture potential. The abbreviations of the amines discussed in each paragraph are reported as a heading so that they can be easily tracked.

#### *Primary amines of Table 4*

##### AMP

The smallest primary amine is a branched molecule rather than the smallest [OCCN] molecule, MEA, which has not been selected as one of the most promising solvents despite its inclusion in the database. In 2-amino-propanol (2AP), 2-amino-1-butanol (2A1B), 2-amino-1-pentanol (2A1PN) and 2-amino-1-hexanol (2A1H) the  $\alpha$ -carbon hydrogen atom of MEA is substituted by a carbon chain which generally increases the steric hindrance. This is even more pronounced in 2-amino-2-methyl-1-propanol (AMP) which is a well-known sterically-hindered amine. AMP is one of the most investigated amines in CO<sub>2</sub> capture literature and has been tested in a pilot unit as the solvent of choice in a mixture with piperazine in the CESAR project<sup>48</sup>.

##### 2A1B, 2A1PN, 2A1H

2A1B, 2A1PN and 2A1H have been considered in mixtures with methyldiethanolamine (MDEA-R16) where they were tested experimentally in terms of stability and corrosiveness with respect to carbon steel<sup>69</sup>. The tests were motivated by the discovery that an aqueous mixture comprising

a tertiary alkanolamine and a primary alkanolamine with a secondary carbon atom attached to the amino group (such as 2A1B, 2A1PN and 2A1H) is not only effective in removing acidic gases but it also exhibits unexpectedly low degradation, corrosiveness and metals solubility properties. 2A1B was found to exhibit very high stability and low corrosiveness, performing much better than ethylaminoethanol (EMEA) and butylmonoethanolamine (BMEA)<sup>69</sup>.

### 2AP, MIPA, MDEA

2AP was investigated by Da Silva<sup>47</sup> who reported a carbamate stability close to that of MEA. If the methyl group is moved to the  $\beta$ -carbon atom, the structure becomes 1-amino-2-propanol (MIPA)<sup>75</sup> which presents  $\text{CO}_2$  solubility behaviour very similar to MDEA at the same concentration, and much higher than MEA, diethanolamine (DEA) and diisopropanolamine (DIPA)<sup>77</sup>. MDEA is a sterically hindered amine of high industrial interest due to increased absorption capacity and high selectivity towards contaminants such as  $\text{H}_2\text{S}$ <sup>77</sup>. Considering that MDEA has a  $pK_a$  of 8.56 and MIPA of 9.45<sup>75</sup> it is clear that the latter is likely to exhibit much faster kinetics. Note that MIPA was not in the set of available amines, otherwise it is likely that it might have been identified in the 29 selected solvents. In any case, MIPA was identified here due to its resemblance to 2AP and is therefore worth of further investigation.

### *Secondary amines of Table 4*

#### MMEA, BEA

The molecules in the -NH- row of Table 4 are also based on the same main [OCCN] structure as previously. The pattern that appears toward the right end of each structure, as drawn in the table, results from substitution of a hydrogen atom of the MEA amine group by different carbon chains which gradually increase from left-to-right. 2-(methylamino)-ethanol (MMEA) has a slightly higher absorption rate than MEA at low loadings and considerably outperforms MEA at higher loadings<sup>49</sup>. MMEA also has a somewhat higher molecular weight and therefore, a lower molar concentration. In addition, MMEA has a moderate carbamate stability resulting in increased absorbed amounts of  $\text{CO}_2$  at low partial pressure. Both MMEA and 2-(butylamino)-ethanol (BEA) exhibit foaming and MMEA is in this respect worse than BEA<sup>49</sup>.

#### EMEA, PAE

Ethylaminoethanol (EMEA) is also a well-known secondary amine which exhibits considerably higher  $\text{CO}_2$  loadings than MEA, DEA and MMEA (at 30% w/w) over a wide range of pressures<sup>50</sup>. 2-Propylamino-ethanol (PAE) exhibits much higher  $\text{CO}_2$  loadings than MEA and higher  $\text{CO}_2$  cyclic capacity than both MEA and DEA<sup>70</sup>. At 30 wt% and 313K EMEA exhibits a  $\text{CO}_2$  loading of over 0.9 after approximately 75 kPa of pressure with a tendency to rise up to 1.5 mole/ $\text{CO}_2$  mole amine at 550 kPa<sup>50</sup>. At the same specifications PAE exhibits a  $\text{CO}_2$  loading slightly over 0.8, with a similar tendency to rise<sup>70</sup>. A comparative study by Yamada et al.<sup>2</sup> of EMEA, PAE and BEA indicates that they all exhibit relatively similar  $\text{CO}_2$  loadings which are mainly affected by the length of the hydroxyl chain (i.e. at the left end of the amine nitrogen).

### IPAE, 1M2P

2-(Isopropylamino)-ethanol (IPAE) is very similar to PAE, exhibiting slightly higher CO<sub>2</sub> loadings due to increased steric hindrance, but lower reaction rates<sup>70</sup>. The structure of 1-methylamino-propan-2-ol (1M2P) is very similar to MMEA with the addition of a methyl group next to the hydroxyl, which makes the hydroxyl attached to a  $\beta$ -carbon atom with respect to the amine. This is likely to follow the heuristic of Structure-Property Relation (3) in Table 1 when 1M2P is compared with MMEA.

### DIBA, DsBA, DIPA

Diisobutylamine (DIBA) and Di-sec butylamine (DsBA)<sup>71, 72</sup> belong to the important class of thermomorphic biphasic solvents (TBS), comprising lipophilic amines as the active components which exhibit a liquid–liquid phase separation (LLPS) upon heating. This enables the non-thermal extraction of a lean CO<sub>2</sub> phase prior to desorption which may take place at much lower temperatures than the 120°C of conventional systems. The low regeneration temperature of often less than 90°C together with the high cyclic CO<sub>2</sub> loading capacity considerably reduces the energetic desorption requirements. Furthermore, low-grade heat (e.g. recovered from a waste heat stream) may be used as an option instead of steam, whereas solvent degradation is typically lower at lower temperatures. The results from experimental investigations of DIBA indicate fast kinetics up to a CO<sub>2</sub> loading of approximately 0.6-0.65 mol/mol amine, which is the maximum capacity achieved<sup>71, 72</sup>. The very similar Diisopropylamine (DIPA)<sup>71</sup> exhibits fast kinetics up to a loading of approximately 0.9 mol/mol amine. Note that DIPA was not on our set of examined amines. From a structural perspective DIBA and DsBA fall into Structure-Property relation (5). DsBA is very similar to DIBA except that the two side methyl groups have been moved to the  $\alpha$ -carbon after the amine. This is a useful option because the undesired insoluble carbamate salts formation associated with DIBA may be avoided while the reaction kinetics may be improved due to the branching moved to the  $\alpha$ -carbon<sup>71</sup>. DsBA is considered an interesting regeneration promoter with a liquid–liquid phase separation temperature for the 3M solution at 60°C and over 95% regenerability at 80°C.

### ***Tertiary amines of Table 4***

#### DMMEA

N,N-Dimethylaminoethanol (DMMEA) is a tertiary amine with exactly the same type and number of functional groups as AMP, except that the -CH<sub>3</sub> branch is not on the  $\alpha$ -carbon. Instead, it is directly connected to the nitrogen atom, which leaves no hydrogen atom on the amine functional group. This eliminates the possibility of carbamate formation between the DMMEA and CO<sub>2</sub>, which has two direct effects on the amine properties<sup>51</sup>. Compared with primary and secondary amines, DMMEA has larger absorption capacity, while the energy required to reverse the amine-CO<sub>2</sub> reaction is lower for DMMEA than for amines which can form carbamate with CO<sub>2</sub>. As a tertiary amine it has a low absorption rate so it can be used with an additional activator (i.e., rate promoter).

### DEEA, DPE

N,N-Diethylethanolamine (DEEA) can be considered as a promising absorbent. It includes two ethyl groups replacing the hydrogen atoms of the amino group in MEA, it reacts slowly with CO<sub>2</sub> because of its tertiary amine characteristics but enables high CO<sub>2</sub> loading capacity<sup>52</sup>. Di-N-Propylethylamine (DPE) is structurally very similar to Tributylamine (TBA) and only differs by one –CH<sub>2</sub> group. TBA is reported to result in low loadings<sup>5</sup> hence a similar behavior may be expected.

### ***Primary and secondary amines of Table 5***

#### MPA, DBA

The structures in Table 5 follow a similar pattern as those in Table 4 but including molecules of the structural types [OCCCN] or [CCCCN]. Structure [OCCCN] is in line with Structure-Property Relation (1) in Table 1. 3-Amino-1-propanol (MPA-R8) is one carbon atom longer, reacts faster with CO<sub>2</sub><sup>53</sup> and has increased absorption capacity compared to MEA<sup>78</sup>. Recently, MPA has been patented in a mixture with AMP<sup>79</sup> which combines the faster kinetics of MPA with the favourable regeneration and CO<sub>2</sub> solubility features of AMP. Additional major advantages of this mixture compared to either MEA or MEA with AMP include reduced oxidative degradation, corrosiveness and formation of nitrosamines. 4-amino-2-butanol (4A2B) is exactly one carbon atom longer than MIPA<sup>75</sup> hence it may reasonably be expected that it will exhibit a similar performance. It exhibits a hydroxyl group three carbon atoms away from the amino nitrogen hence it falls within Structure-Property Relation (1). Di-N-Butylamine (DBA) is also known as a biphasic solvent<sup>71</sup>.

### ***Tertiary amines of Table 5***

#### 3DAP, 3DMA1P, ND1B, 1EDB

The closest structure to 3-(diethyl-amino)-propanol (3DAP) which has been considered as a CO<sub>2</sub> capture option is 3-dimethyl-amino-1-propanol (3DMA1P), which has been shown to exhibit favourable reaction kinetics compared to MDEA<sup>76</sup>. 4-diethylamino-2-butanol (DEAB) is an interesting amine, designed specifically based on Structure-Property Relation (1) to exhibit higher CO<sub>2</sub> capacity, improved reaction rates and lower regeneration energy than MDEA<sup>54</sup>. N,N-Diethyl-1-Butanamine (ND1B) is similar to DPE and also to 3DAP, where the hydroxyl is replaced by a methyl group. ND1B is expected to exhibit lower CO<sub>2</sub> absorption capacity than 3DAP due to the absence of hydroxyl and also low reaction rate because it is a tertiary amine. 1-Ethyl-N,N-dimethylbutylamine (1EDB) appears to exhibit increased steric hindrance due to the bulky constituents around the amino nitrogen which may support CO<sub>2</sub> absorption capacity.

#### TMEDA, 2P12P

The last 2 amines in Table 5 have completely different structural characteristics compared to other solvents. N,N,N',N'-tetramethyl-1,2-Ethanediamine (TMEDA) has been considered in published literature (Bouzina et al., 2012) in a work that investigated experimental VLE in mixtures of this solvent with water while no work is mentioned regarding VLE of this solvent with water and CO<sub>2</sub>. N,N,N',N',2-pentamethyl-1,2-propanediamine (2P12P) is structurally

similar with TMEDA, except that 2 methyl groups replace the hydrogen atoms in the a-carbon atom after the amine group. These 2 groups are likely to increase steric hindrance, while both amines will improve in terms of basicity and desorption capacity by increasing the chain length between the amine groups according to Structure-Property Relation (2).

### *Amines of Table 6*

#### 4AP, 4D1B

Table 6 contains amines of longer chains but of similar structural characteristics as the amines in Tables 4 and 5. 4-amino-pentanol (4AP) appears to be very similar with 2AP. The longer chain of 4 carbon atoms implies an improved desorption capacity compared to 2AP, based on Structure-Property Relation (4). 5-amino-penanol (5AP) is one amine used in the experiments reported in Singh et al.<sup>6, 7, 74</sup> hence it is expected to have lower absorption and desorption capacities compared to hydroxyl-amines of three and four carbons atoms. 4-(Dimethylamino)-1-butanol (4D1B) is very similar to the previously discussed 3DMA1P<sup>76</sup>, with the previous insights regarding the chain lengths also likely to apply in this case.

#### HEXA

Hexanamine (HEXA) has been investigated experimentally on several occasions<sup>6, 7, 71</sup> leading to the conclusion that it exhibits very high absorption capacity and high absorption rates compared to very similar molecules like Heptylamine and Octylamine. It is an interesting phase-change solvent which exhibits liquid-liquid phase separation temperature of 90°C (3 M solution) and regenerability of 40% at 80°C<sup>80</sup>. Together with the high absorption rate, these characteristics make it a useful absorption activator in mixtures with regenerator promoters like DsBA. On the other hand, cyclic variants of HEXA like N,N-Dimethyl Cyclohexylamine (DMCA) have been experimentally studied in Zhang et al.<sup>71</sup>, indicating increased absorption capacity and ability for very good desorption at 90°C.

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