Carbon dioxide post combustion capture: a novel screening study of the carbon dioxide absorption performance of 76 amines

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Figure S1-S 1 Experimental setup used for the determination of CO_2 absorption by isothermal gravimetric analysis.

Figure S1-S 2 (a) Micro-scale evaporation run for 30% w/w MEA. (b) Micro-scale absorption run for 30% MEA. (c) Graph resulting from subtraction of evaporation run from absorption run for 30% MEA.

Figure S1-S 3 Experimental setup used to measure CO_2 absorption on a 300 mL or 20 mL solution volume.

Figure S1-S 4 Plot of the absorption capacity versus amine group pK_a (most basic amine for polyamines) at 40°C. MEA is labelled as a black dot. The eight amines showing outstanding performance are also labelled. The dashed line represents model predictions of absorption capacity as a function of pK_a if only the pathway of Eq. 1 occurs (with a large stability constant and small pK_a for carbamaic acid) and the dotted line if only the pathway of Eq. 2 occurs. The numbering corresponds to Tables S1-S1 to S1-S4.

Figure S1-S 5 Plot showing the initial absorption rate versus amine group pK_a calculated from the IGA micro-scale data. The numbering corresponds to Tables S1-S1 to S1-S4.

Table S1-S 1 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all primary amines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

Table S1-S 2 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all secondary amines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

Table S1-S 3 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all tertiary amines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

Table S1-S 4 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all mixed type polyamines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

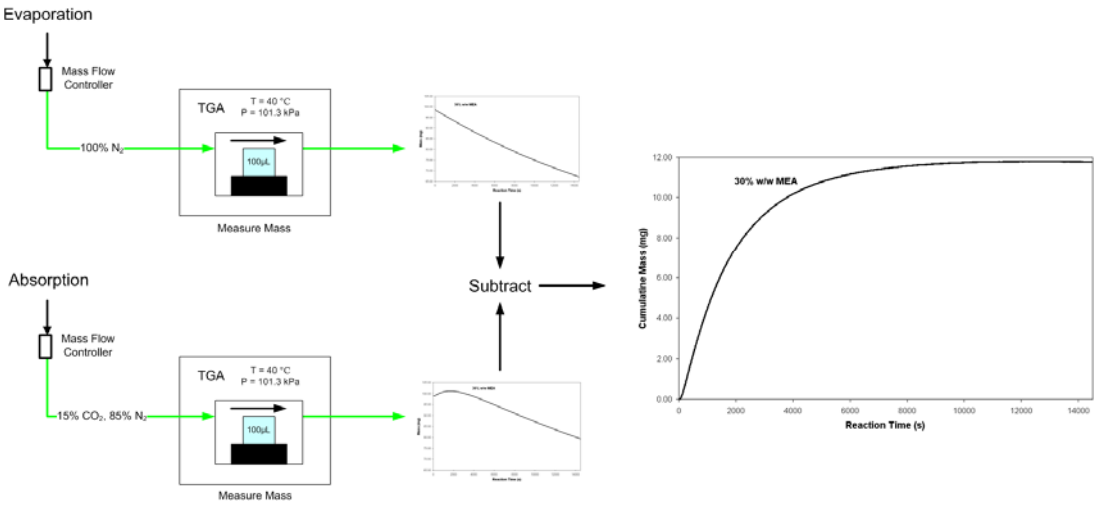


Figure S1-S 1 Experimental setup used for the determination of CO_2 absorption by isothermal gravimetric analysis.

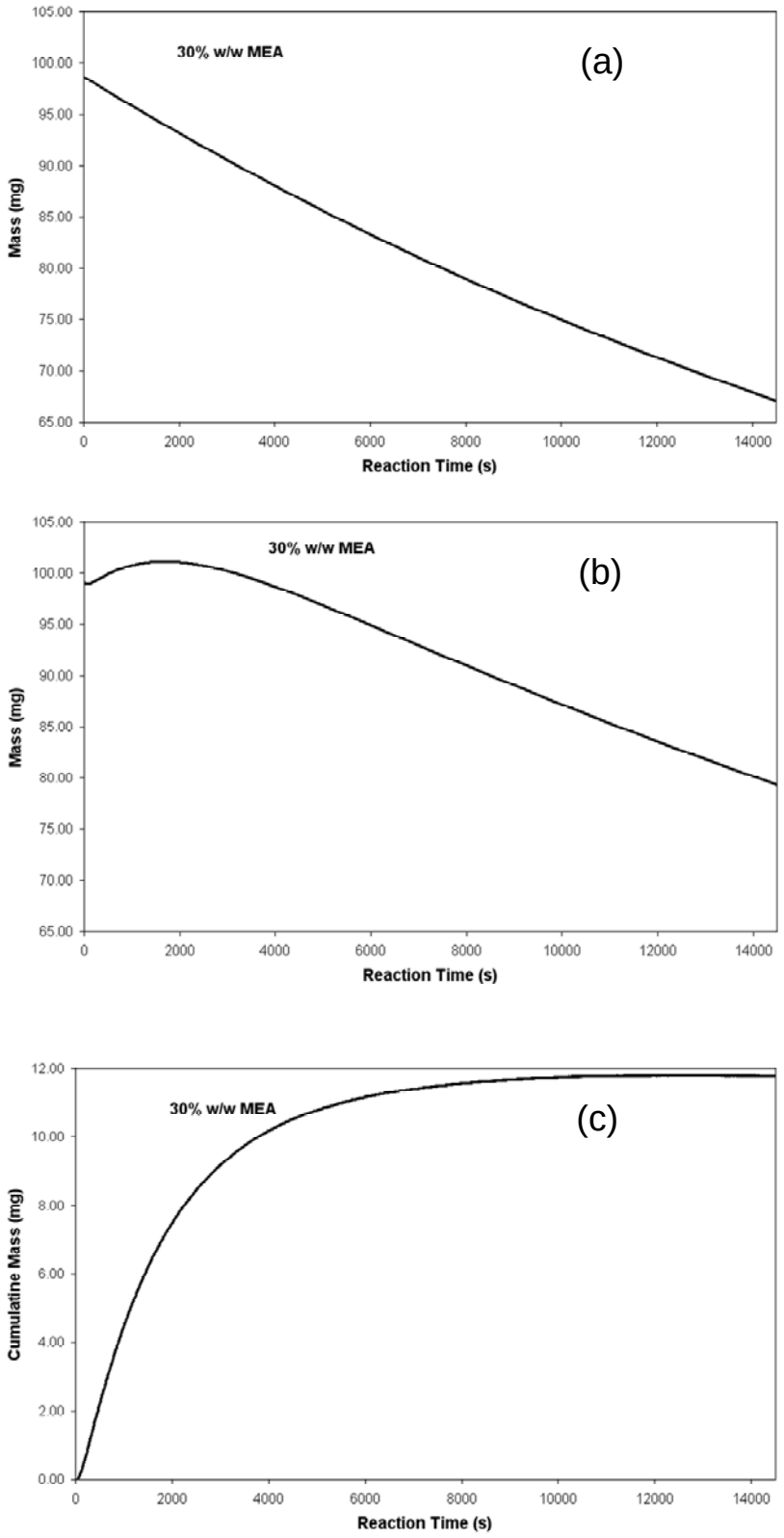


Figure S1-S 2 (a) Micro-scale evaporation run for 30% w/w MEA. (b) Micro-scale absorption run for 30% MEA. (c) Graph resulting from subtraction of evaporation run from absorption run for 30% MEA.

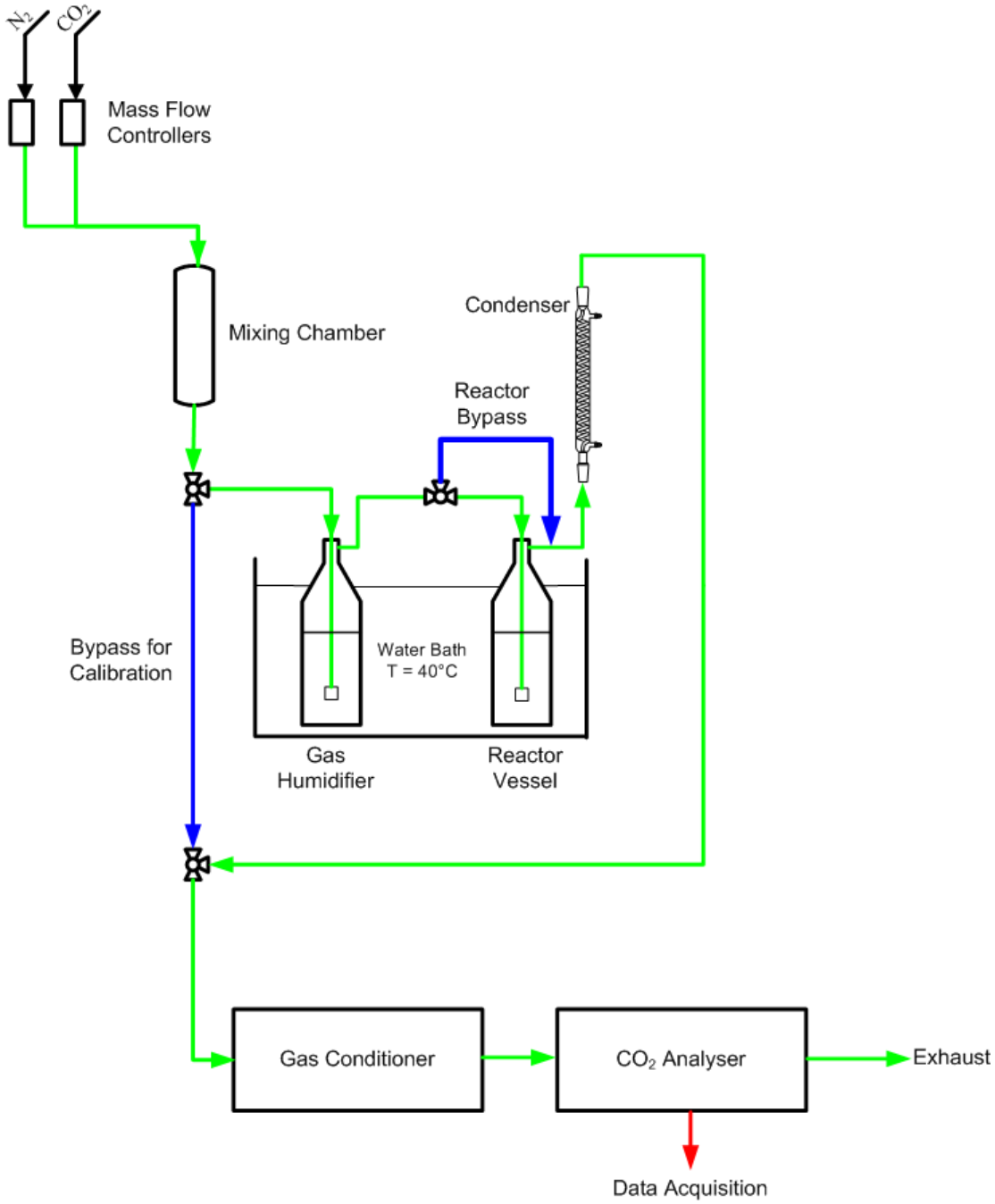
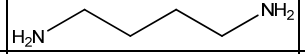
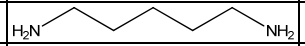
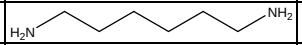
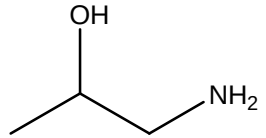
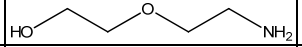
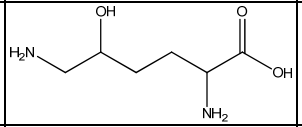
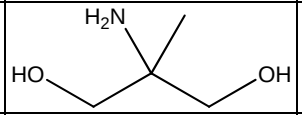
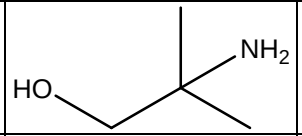
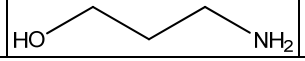
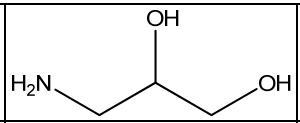
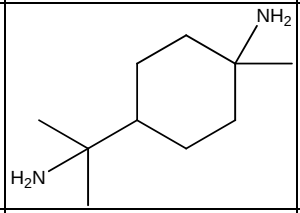
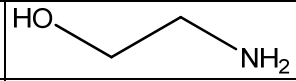
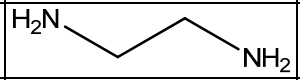
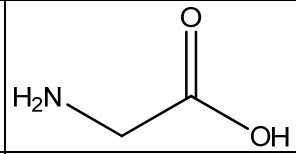
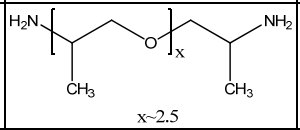
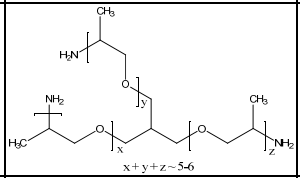
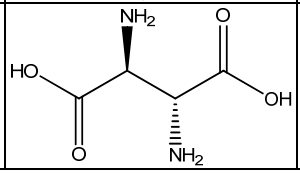
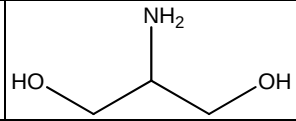
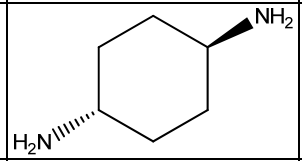
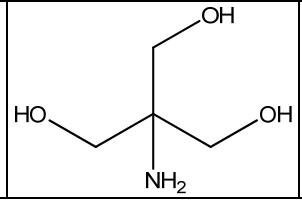


Figure S1-S 3 Experimental setup used to measure CO_2 absorption on a 300 mL or 20 mL solution volume.

Table S1-S 1 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all primary amines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

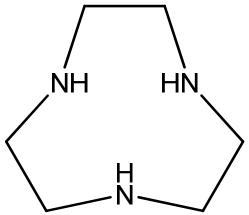
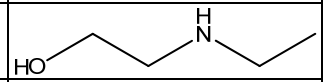
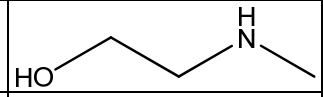
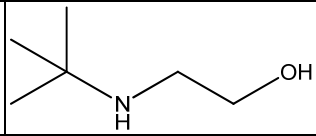
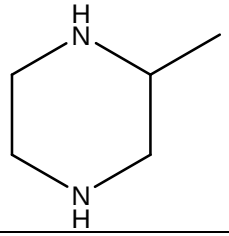
	Amine Number and Name		Amine Structure	Micro-scale / Macro-scale Absorption Capacity (n_{CO2} / n_N)	Micro-scale / Macro-scale Absorption Capacity (g_{CO2} / g_{amine})	Initial Rate (n_{CO2} / n_{amine}, min^{-1})	pK_a at 25°C and I = 0M[#]
Primary Amines	1	1,3-diaminopropane		0.46 / NR	0.54 / NR	0.017	10.4[‡]
	2	1,4-diaminobutane		0.41 / NR	0.41 / NR	0.015	10.3[†]
	3	1,5-diaminopentane		0.45 / NR	0.39 / NR	0.021	10.9[‡]
	4	1,6-diaminohexane		0.45 / NR	0.32 / NR	0.017	10.9[‡]
	5	1-amino-2-propanol		NA / 0.60	NA / 0.35	NA	9.50[†]
	6	2-(2-aminoethoxy)-ethanol		NA / 0.60	NA / 0.25	NA	9.42[†]
	7	2,6-diamino-5-hydroxyhexanoic acid		0.15 / NR	0.06 / NR	0.004	9.02[‡]
	8	2-amino-2-methyl-1,3-propanediol		NA / 0.69	NA / 0.29	NA	8.84[†]
	9	2-amino-2-methyl-1-propanol		0.49 / 0.59 (0.667)[1]	0.24 / 0.29	0.006	9.82[†]
	10	3-amino-1-propanol		NA / 0.56	NA / 0.33	NA	10.0[†]

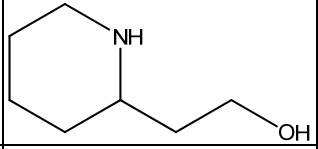
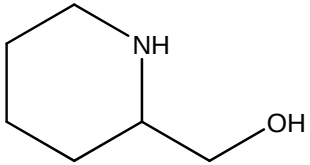
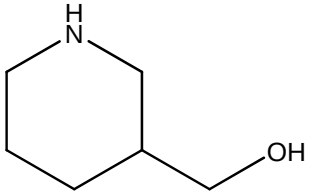
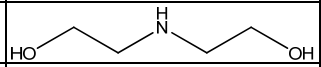
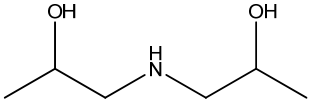
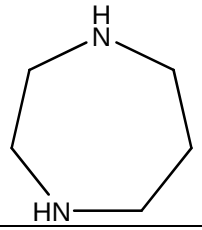
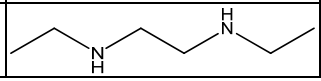
	11	3-aminopropan-1,2-diol		0.46 / NR	0.22 / NR	0.011	8.44‡
	12	4-(2-aminopropan-2-yl)-1-methylcyclohexanamine		NA / 0.25	NA / 0.13	NA	11.0‡
	13	ethanolamine		0.49 / 0.56 (0.558)[2]	0.35 / 0.42	0.014	9.5†
	14	ethylenediamine		0.40 / 0.50	0.59 / 0.8	0.014	9.93†
	15	glycine		0.27 / NR	0.16 / NR	0.003	9.78†
	16	Jeffamine D230		0.45 / NR	0.18 / NR	0.021	9.14‡×
	17	Jeffamine T403		0.33 / NR	0.10 / NR	0.015	9.29‡×
	18	meso-2,3-diaminosuccinic acid		0.32 / NR	0.22 / NR	0.032	10.9‡

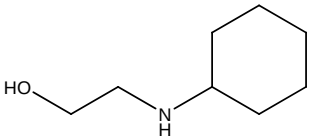
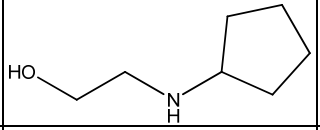
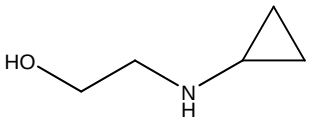
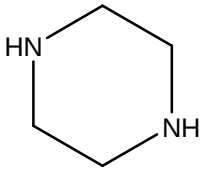
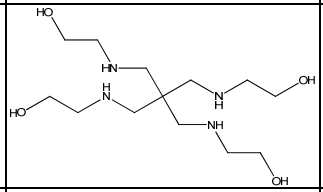
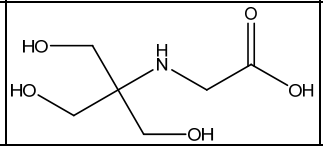
	19	pentan-1-amine		NA / 0.77	NA / 0.39	NA	10.7[†]
	20	serinol (2-aminopropane-1,3-diol)		0.48 / NR	0.23 / NR	0.011	8.55[‡]
	21	trans-1,4-diaminocyclohexane		0.50 / NR	0.38 / NR	0.016	10.8[‡]
	22	tris(hydroxymethyl)amino methane		0.33 / 0.28	0.12 / 0.10	0.0029	8.08[†]

NA – Experimental results not available due to excessive evaporation or precipitation.
NR – Experiments with this amine were not run in the apparatus.
[#] The listed pK_a is for the amine group or most basic amine group for polyamines.
[×] The pK_a calculation is based on one unit of the polymer.
[†] Source - NIST *NIST Critically Selected Stability Constants of Metal Complexes*, The National Institute of Standards and Technology: Gaithersburg, 2001.
[‡] Calculated using - ACD/I-Lab ACD/pK_a 8.3. http://ilab.acdlabs.com/.

Table S1-S 2 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all secondary amines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

	Amine Number and Name		Amine Structure	Micro-scale / Macro-scale Absorption Capacity (n_{CO2} / n_N)	Micro-scale / Macro-scale Absorption Capacity (g_{CO2} / g_{amine})	Initial Rate (n_{CO2} / n_{amine}, min^{-1})	pK_a at 25°C and I = 0M[#]
Secondary Amines	23	1,4,7-triazacyclononane*		0.27 / NR	0.28 / NR	0.029	10.6[‡]
	24	2-(ethylamino)ethanol		0.61 / 0.77 (~0.58)[3]	0.30 / 0.38	0.010	10.0[†]
	25	2-(methylamino)ethanol		0.58 / 0.63 (~0.51)[3]	0.34 / 0.37	0.012	9.88[†]
	26	2-(tert-butylamino)ethanol		0.40 / NR (~0.55)[3]	0.15 / NR	0.005	9.70[‡]
	27	2-methylpiperazine		0.35 / NR	0.31 / NR	0.010	5.64[‡]

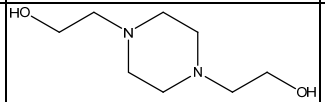
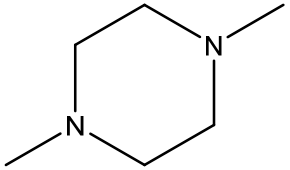
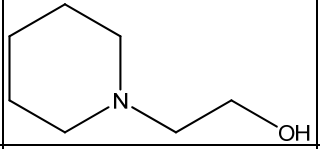
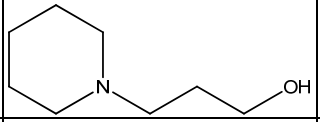
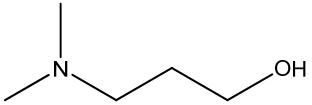
	28	2-piperidineethanol		1.0 / 1.0	0.35 / 0.35	0.011	10.9[‡]
	29	2-piperidinemethanol		1.0 / NR	0.37 / NR	0.012	10.6[‡]
	30	3-piperidinemethanol		0.8 / NR	0.30 / NR	0.013	10.8[‡]
	31	diethanolamine		0.53 / 0.60 (0.548)[1]	0.22 / 0.25	0.008	8.88[†]
	32	diisopropanolamine		NA / 0.64 (0.446)[4]	NA / 0.21	NA	8.88[†]
	33	homopiperazine		0.70 / NR	0.61 / NR	0.045	11.0[‡]
	34	N,N'-diethylethylenediamine		NA / 0.45	NA / 0.35	NA	10.1[†]

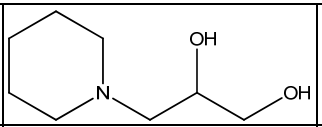
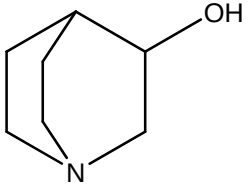
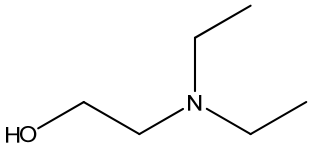
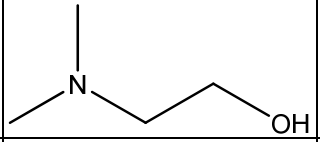
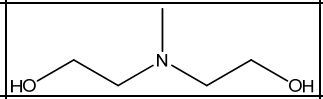
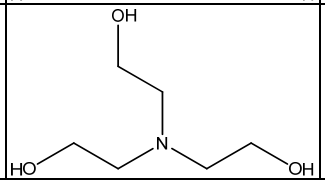
	35	N-cyclohexylethanolamine		0.52 / NR	0.16 / NR	0.005	10.1‡
	36	N-cyclopentylethanolamine		0.74 / NR	0.25 / NR	0.007	10.1‡
	37	N-cyclopropylethanolamine		0.46 / NR	0.20 / NR	0.006	8.40‡
	38	piperazine		0.65 / 0.55 (0.523)[5]	0.65 / 0.58	0.031	9.73†
	39	tetrakis(2-hydroxyethylaminomethyl)methane		0.28 / NR	0.16 / NR	0.016	9.53‡
	40	tricine		0.10 / NR	0.023 / NR	0.004	8.10†

NA – Experimental results not available due to excessive evaporation or precipitation.
NR – Experiments with this amine were not run in the apparatus.
[#] The listed pK_a is for the amine group or most basic amine group for polyamines.
* Only a 10% w/w aqueous solution due to low solubility.

† Source - NIST *NIST Critically Selected Stability Constants of Metal Complexes*, The National Institute of Standards and Technology: Gaithersburg, 2001.
‡ Calculated using - ACD/I-Lab ACD/pK_a 8.3. http://ilab.acdlabs.com/.

Table S1-S 3 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all tertiary amines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

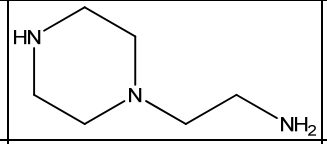
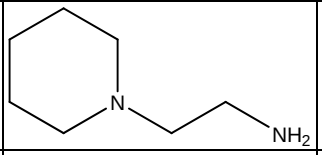
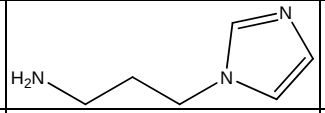
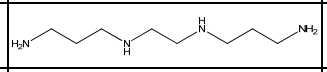
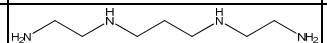
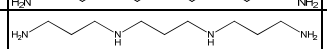
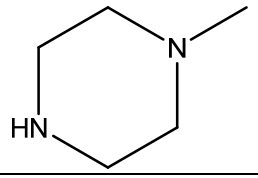
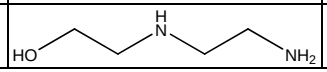
		Amine Name	Amine Structure	Micro-scale / Macro-scale Absorption Capacity (n_{CO2} / n_N)	Micro-scale / Macro-scale Absorption Capacity (g_{CO2} / g_{amine})	Initial Rate (n_{CO2} / n_{amine}, min^{-1})	pK_a at 25°C and I = 0M[#]
Tertiary Amines	41	1,4-bis(2-hydroxyethyl) piperazine		0.25 / NR	0.12 / NR	0.003	6.62[‡]
	42	1,4-dimethylpiperazine		0.07 / NR	0.05 / NR	0.002	8.61[‡]
	43	1-piperidineethanol		0.26 / 0.28	0.09 / 0.10	0.004	9.04[‡]
	44	1-piperidinepropanol		0.46 / NR	0.14 / NR	0.004	9.43[‡]
	45	3-dimethylamino-1-propanol		0.14 / NR	0.06 / NR	0.001	9.27[‡]

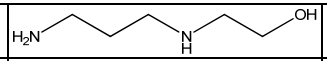
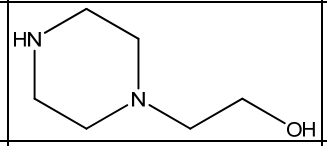
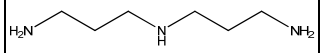
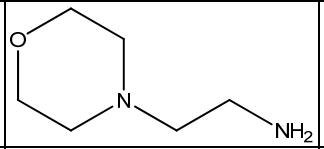
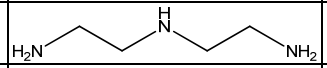
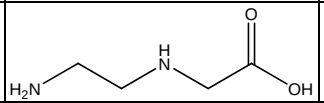
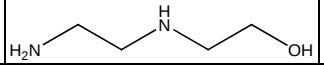
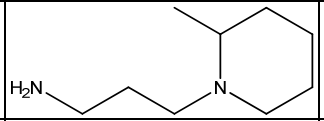
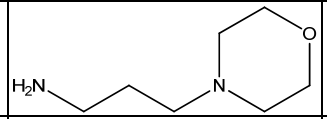
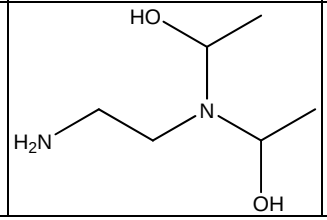
	46	3-piperidino-1,2-propanediol		1.1 / NR	0.30 / NR	0.008	8.91‡
	47	3-quinuclidinol		1.1 / NR	0.38 / NR	0.004	10.1‡
	48	N,N-diethylethanolamine		0.69 / NR	0.26 / NR	0.004	9.79‡
	49	N,N-dimethylethanolamine		NA / 0.92	NA / 0.35	0.002	9.57†
	50	N-methyldiethanolamine		0.40 / NR (0.441)[6]	0.15 / NR	0.003	8.63†
	51	triethanolamine		NA / 0.24	NA / 0.07	NA	7.76†

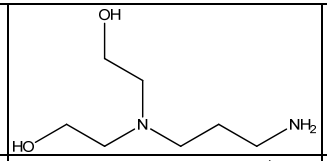
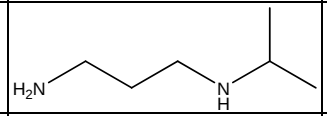
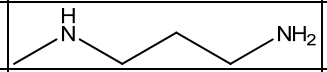
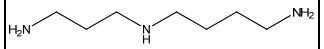
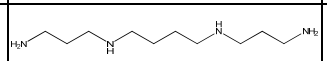
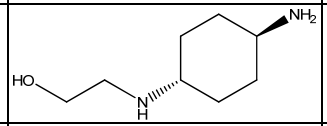
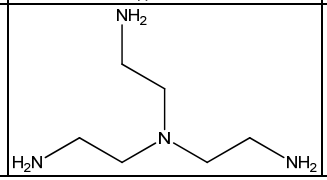
NA – Experimental results not available due to excessive evaporation or precipitation.
NR – Experiments with this amine were not run in the apparatus.
The listed pK_a is for the amine group or most basic amine group for polyamines.
† Source - NIST *NIST Critically Selected Stability Constants of Metal Complexes*, The National Institute of Standards and Technology: Gaithersburg, 2001.

‡ Calculated using - ACD/I-Lab ACD/pK_a 8.3. http://ilab.acdlabs.com/.

Table S1-S 4 The chemical name, chemical structure normalised molar CO_2 absorption capacity (micro-scale and macro-scale apparatus), CO_2 absorption capacity on a mass basis, initial absorption rate and pK_a of all mixed type polyamines. Literature data of absorption capacity measured under comparable conditions is given in parentheses where available. The experimental results are for 30% w/w aqueous solutions at 40°C, ambient pressure and a gas composition of 15% CO_2 (micro-scale) or 13% CO_2 (macro-scale) with the balance N_2.

		Amine Name	Amine Structure	Micro-scale / Macro-scale Absorption Capacity (n_{CO2} / n_N)	Micro-scale / Macro-scale Absorption Capacity (g_{CO2} / g_{amine})	Initial Rate (n_{CO2} / n_{amine}, min^{-1})	pK_a at 25°C and I = 0M[#]
Mixed Type Polyamines	52	1-(2-aminoethyl)piperazine		0.23 / NR	0.22 / NR	0.014	10.1[‡]
	53	1-(2-aminoethyl)piperidine		0.55 / NR	0.38 / NR	0.013	10.2[‡]
	54	1-(3-aminopropyl)imidazole		0.17 / NR	0.19 / NR	0.013	9.08[‡]
	55	1,2-bis(3-aminopropylamino)ethane		0.35 / NR	0.35 / NR	0.019	10.5[‡]
	56	1,4,8,11-tetraazaundecane		0.33 / NR	0.36 / NR	0.019	10.2[‡]
	57	1,5,9,13-tetraazatridecane		0.40 / NR	0.37 / NR	0.020	10.5[‡]
	58	1-methylpiperazine		0.32 / NR	0.28 / NR	0.010	9.65[‡]
	59	2-(2-aminoethylamino)ethanol		0.48 / 0.55 (0.446)[7]	0.40 / 0.46	0.014	9.76[†]

	60	2-(3-aminopropylamino)ethanol		0.59 / 0.60	0.44 / 0.45	0.018	10.4[†]
	61	2-piperazin-1-ylethanol		0.33 / NR	0.22 / NR	0.010	9.27[‡]
	62	3,3-iminodipropylamine or bis(3-aminopropyl)amine		0.37 / NR	0.44 / NR	0.016	10.5[‡]
	63	4-(2-aminoethyl)morpholine		0.30 / NR	0.20 / NR	0.013	9.93[‡]
	64	diethylenetriamine		NA / 0.59	NA / 0.75	0.016	9.93[†]
	65	N-(2-aminoethyl)glycine		0.25 / NR	0.18 / NR	0.009	9.82[‡]
	66	N-(2-hydroxyethyl)ethylenediamine		0.48 / NR	0.40 / NR	0.017	9.61[‡]
	67	N-(3-aminopropyl)-2-pipecoline		0.45 / NR	0.26 / NR	0.014	10.4[‡]
	68	N-(3-aminopropyl)morpholine		0.28 / NR	0.17 / NR	0.010	10.3[‡]
	69	N,N-bis(1-hydroxyethyl)ethylenediamine		0.55 / NR	0.31 / NR	0.018	9.43[‡]

	70	N,N-bis(hydroxyethyl)-trimethylenediamine		0.25 / NR	0.13 / NR	0.009	10.0‡
	71	N-isopropyl-1,3-propanediamine		0.62 / NR	0.47 / NR	0.015	10.6‡
	72	N-methyl-1,3-propanediamine		0.39 / NR	0.39 / NR	0.016	10.6‡
	73	spermidine (N1-(3-aminopropyl)butane-1,4-diamine)		0.41 / NR	0.37 / NR	0.021	10.5‡
	74	spermine (N1,N1'-(butane-1,4-diyl)dipropane-1,3-diamine)		0.45 / NR	0.40 / NR	0.028	10.9‡
	75	trans-N-hydroxyethyl-1,4-diaminocyclohexane		0.45 / NR	0.24 / NR	0.027	10.5‡
	76	tris(2-aminoethyl)amine		0.30 / NR	0.36 / NR	0.003	10.0‡

NA – Experimental results not available due to excessive evaporation or precipitation.
NR – Experiments with this amine were not run in the apparatus.
The listed pK_a is for the amine group or most basic amine group for polyamines.
† Source - NIST *NIST Critically Selected Stability Constants of Metal Complexes*, The National Institute of Standards and Technology: Gaithersburg, 2001.
‡ Calculated using - ACD/I-Lab ACD/pK_a 8.3. http://ilab.acdlabs.com/.

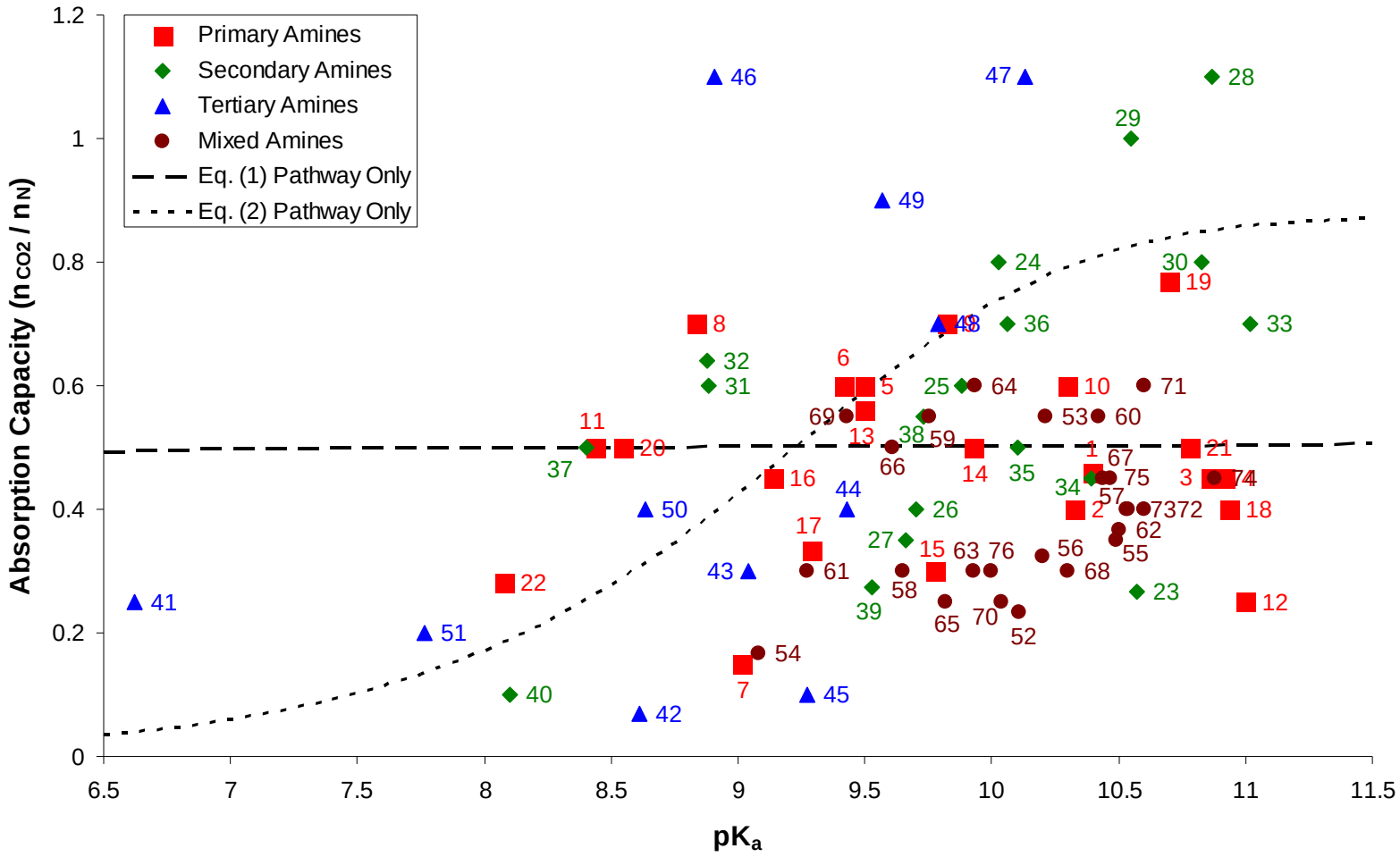


Figure S1-S 4 Plot of the absorption capacity versus amine group pK_a (most basic amine for polyamines) at 40°C. MEA is labelled as a black dot. The eight amines showing outstanding performance are also labelled. The dashed line represents model predictions of absorption capacity as a function of pK_a if only the pathway of Eq. 1 occurs (with a large stability constant and small pK_a for carbamaic acid) and the dotted line if only the pathway of Eq. 2 occurs. The numbering corresponds to Tables S1-S1 to S1-S4.

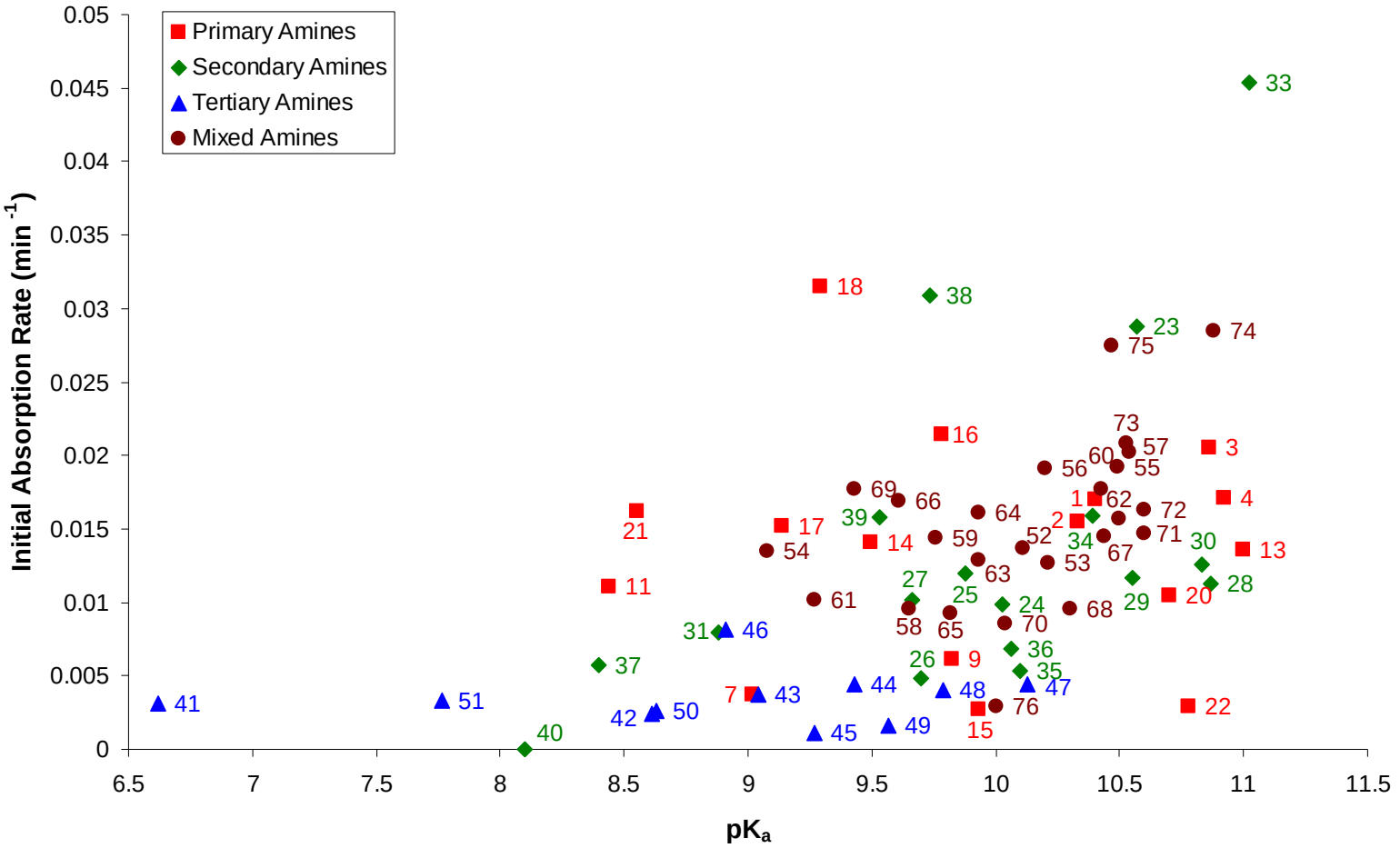


Figure S1-S 5 Plot showing the initial absorption rate versus amine group pK_a calculated from the IGA micro-scale data. The numbering corresponds to Tables S1-S1 to S1-S4.

References

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