Appendix A - Preparation of salts and results achieved

Please refer to Section 3.2 of Materials and Methods for an explanation of the crystallisation methods utilised for salt synthesis. The tables below detail the synthesis of all salts prepared, with their crystallisation method and the outcome of the synthesis. Where single crystal analysis was performed previously the database reference is stated.

Table A.1 Attepmted synthesis of phenethylammonium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
PEA2CB	1.00 ml, 7.96 mmol	1.3713 g, 8.76 mmol	1	amorphous solid
PEA2FB	1.00 ml. 7.96 mmol	1.2246 g, 8.74 mmol	1	amorphous solid
PEA2HB	1.00 ml, 7.96 mmol	1.2070 g, 8.74 mmol	10	oil
PEA3CB	1.00 ml, 7.96 mmol	1.3711 g, 8.76 mmol	1	crystals **PEA3CB**
PEA3FB	1.00 ml, 7.96 mmol	1.2240 g, 7.74 mmol	1	crystals **PEA3FB**
PEA4CB	1.00 ml, 7.96 mmol	1.3711 g, 8.76 mmol	3	crystals
PEA4FB	1.00 ml, 7.96 mmol	1.2258 g, 8.75 mmol	1	crystals **PEA4FB**
PEA4HB	1.00 ml, 7.96 mmol	1.0939 g, 7.92 mmol	1	crystals **PEA4HB**
PEA4HBS	1.00 ml, 7.96 mmol	2.34 ml, 8.72 mmol	1	crystals **PEA4HBS**
PEAAdp	1.00 ml, 7.96 mmol	1.2741 g, 8.72 mmol	3	poor crystals
PEABF4	1.00 ml, 7.96 mmol	1.53 ml, 8.72 mmol	1	crystals **PEABF4**
PEABr	1.00 ml, 7.96 mmol	1.47 ml, 8.72 mmol	1	crystals**ZZZOSE01**[1]
PEABS	1.00 ml, 7,96 mmol	1.2689 g, 8.02 mmol	2	poor crystals
PEACl	1.00 ml, 7.96 mmol	0.86 ml, 8.76 mmol	1	crystals **PEAHCL01**[2]
PEAClO4	1.00 ml, 7.96 mmol	1.25 ml, 8.72 mmol	1	poor crystals
PEAEDS	1.00 ml, 7.96 mmol	1.5103 g, 7.94 mmol	1	crystals **PEAEDS**
PEAEtSO3	1.00 ml, 7.96 mmol	1.38 ml, 8.72 mmol	1	crystals **PEAEtSO3**
PEAFum	1.00 ml, 7.96 mmol	1.0154 g, 8.75 mmol	1	crystals **COCPEQ**[3]
PEAI	1.00 ml, 7.96 mmol	1.31 ml, 8.72 mmol	2	poor crystals
PEALMal	1.00 ml, 7.96 mmol	1.1714 g, 8.74 mmol	2	oil
PEALMD	1.00 ml, 7.96 mmol	1.3318 g, 8.75 mmol	1	crystals **PEALMD**
PEALTar	1.00 ml, 7.96 mmol	1.3187 g, 8.79 mmol	2	poor crystals
PEAMale	1.00 ml, 7.96 mmol	0.9292 g, 8.01 mmol	1	crystals **PEAMale**
PEAMalon	1.00 ml, 7.96 mmol	0.8557 g, 8.22 mml	2	crystals **PEAMalon**
PEAMeSO3	1.00 ml, 7.96 mmol	1.20 ml, 8.72 mmol	1	crystals **PEAMeSO3**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
PEAoTol	1.00 ml, 7.96 mmol	1.1959 g, 8.78 mmol	3	crystals
PEAPO4	1.00 ml, 7.96 mmol	1.01 ml, 8.72 mmol	1	poor crystals
PEApTol	1.00 ml, 7.96 mmol	1.1944 g, 8.77 mmol	1	crystals **PEApTol**
PEARMal	1.00 ml, 7.96 mmol	1.1724 g, 8.74 mmol	1	crystals **PEARMal**
PEARMD	1.00 ml, 7.96 mmol	1.2165 g, 7.99 mmol	1	crystals **PEARMD**
PEARTar	1.00 ml, 7.96 mmol	1.1979 g, 7.98 mmol	1	crystals **PEARTar**
PEASO4	1.00 ml, 7.96 mmol	0.83 ml, 8.72 mmol	1	crystals **PEASO4**
PEASuc	1.00 ml, 7.96 mmol	1.0321 g, 8.74 mmol	1	crystals **COCPIU**[3]

Table A.2 Attempted synthesis of methylphenethylaminium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
MPEA2CB	1.00 ml, 6.88 mmol	1.1872 g, 7.60 mmol	1	crystals **MPEA2CB**
MPEA2FB	1.00 ml, 6.88 mmol	1.0656 g, 7.60 mmol	10	oil
MPEA2HB	1.00 ml, 6.88 mmol	1.0518 g, 7.61 mmol	1	crystals **MPEA2HB**
MPEA3CB	1.00 ml, 6.88 mmol	1.1850 g, 7.57 mmol	10	oil
MPEA3FB	1.00 ml, 6.88 mmol	1.0686 g, 7.63 mmol	10	oil
MPEA3NB	1.00 ml, 6.88 mmol	1.2633 g, 7.56 mmol	1	crystals **MPEA3NB**
MPEA4CB	1.00 ml, 6.88 mmol	1,1815 g, 7.55 mmol	2	oil
MPEA4FB	1.00 ml, 6.88 mmol	1.0653 g, 7.60 mmol	1	oil
MPEA4HB	1.00 ml, 6.88 mmol	0.9507 g, 6.88 mmol	1	crystals **MPEA4HB**
MPEA4HBS	1.00 ml, 6.88 mmol	1.84 ml, 6.88 mmol	1	crystals **MPEA4HBS**
MPEAAdp	1.00 ml, 6.88 mmol	1.1013 g, 7.53 mmol	1	crystals **MPEAAdp**
MPEABF4	1.00 ml, 6.88 mmol	1.51 ml, 6.88 mmol	1	poor crystals
MPEABr	1.00 ml, 6.88 mmol	1.16 ml, 6.88 mmol	1	poor crystals
MPEABS	1.00 ml, 6.88 mmol	1.0859 g, 6.87 mmol	2	poor crystals
MPEACl	1.00 ml, 6.88 mmol	0.68 ml, 6.88 mmol	1	poor crystals
MPEAClO4	1.00 ml, 6.88 mmol	0.99 ml, 6.88 mmol	1	poor crystals
MPEAEDS	1.00 ml, 6.88 mmol	1.3085 g, 6.88 mmol	1	crystals **MPEAEDS**
MPEAEtSO3	1.00 ml, 6.88 mmol	1.08 ml, 6.88 mmol	1	oil
MPEAFum	1.00 ml, 6.88 mmol	0.8793 g, 7.57 mmol	1	poor crystals
MPEAI	1.00 ml, 6.88 mmol	1.03 ml, 6.88 mmol	2	poor crystals
MPEALMal	1.00 ml, 6.88 mmol	1.0088 g, 7.52 mmol	1	crystals **MPEALMal**
MPEALMD	1.00 ml, 6.88 mmol	1.1534 g, 7.58 mmol	1	poor crystals
MPEALTar	1.00 ml, 6.88 mmol	1.1300 g, 7.53 mmol	1	crystals **MPEALTar**
MPEAMale	1.00 ml, 6.88 mmol	0.8032 g, 6.92 mmol	1	crystals **MPEAMale**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
MPEAMalon	1.00 ml, 6.88 mmol	0.7224 g, 6.94 mmol	1	crystals **MPEAMalon**
MPEAMeSO3	1.00 ml, 6.88 mmol	0.94 ml, 6.88 mmol	1	oil
MPEAoTol	1.00 ml, 6.88 mmol	1.0291 g, 7.56 mmol	2	amorphous solid
MPEAPO4	1.00 ml, 6.88 mmol	0.79 ml, 6.88 mmol	1	crystals **MPEAPO4**
MPEApTol	1.00 ml, 6.88 mmol	1.0308 g, 7.57 mmol	1	oil
MPEARMal	1.00 ml, 6.88 mmol	1.0116 g, 7.54 mmol	1	conglomerate
MPEARMD	1.00 ml, 6.88 mmol	1.0555 g, 6.94 mmol	2	crystals **MPEARMD**
MPEARTar	1.00 ml, 6.88 mmol	1.0321 g, 6.88 mmol	5	poor crystals
MPEASO4	1.00 ml, 6.88 mmol	0.71 ml, 6.88 mmol	1	crystals **MPEASO4**
MPEASuc	1.00 ml, 6.88 mmol	0.8971 g, 7.60 mmol	1	crystals **MPEASuc**

Table A.3 Attempted synthesis of dimethylphenethylaminium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
DMPEA2CB	1.00 ml, 5.96 mmol	1.0212 g, 6.52 mmol	10	oil
DMPEA2FB	1.00 ml, 5.96 mmol	0.9175 g, 6.55 mmol	10	oil
DMPEA2HB	1.00 ml, 5.96 mmol	0.9044 g, 6.55 mmol	1	crystals **DMPEA2HB**
DMPEA3CB	1.00 ml, 5.96 mmol	1.0213 g, 6.52 mmol	10	oil
DMPEA3FB	1.00 ml, 5.96 mmol	0.9184 g, 6.55 mmol	10	oil
DMPEA4CB	1.00 ml, 5.96 mmol	1.0264 g, 6.56 mmol	1	amorphous solid
DMPEA4FB	1.00 ml, 5.96 mmol	0.9153 g, 6.53 mmol	10	oil
DMPEA4HB	1.00 ml, 5.96 mmol	0.8179 g, 5.92 mmol	1	crystals **DMPEA4HB**
DMPEA4HBS	1.00 ml, 5,96 mmol	1.60 ml, 5.96 mmol	3	amorphous solid
DMPEAAdp	1.00 ml, 5.96 mmol	0.9561 g, 6.54 mmol	1	crystals **DMPEAAdp**
DMPEABF4	1.00 ml, 5.96 mmol	1.30 ml, 5.96 mmol	1	liquid
DMPEABr	1.00 ml, 5.96 mmol	1.00 ml, 5.96 mmol	1	poor crystals
DMPEABS	1.00 ml, 5.96 mmol	1.0469 g, 5.96 mmol	1	crystals **DMPEABS**
DMPEACl	1.00 ml, 5.96 mmol	0.59 ml, 5.96 mmol	1	crystals **DMPEACl**
DMPEAClO4	1.00 ml, 5.96 mmol	0.86 ml, 5.96 mmol	1	crystals **DMPEAClO4**
DMPEAEDS	1.00 ml, 5,96 mmol	1.1336 g, 5.96 mmol	1	crystals **DMPEAEDS**
DMPEAEtSO3	1.00 ml, 5.96 mmol	0.94 ml, 5.96 mmol	1	oil
DMPEAFum	1.00 ml, 5.96 mmol	0.7622 g, 6.57 mmol	1	acid formed
DMPEAI	1.00 ml, 5.96 mmol	0.89 ml, 5.96 mmol	1	poor crystals
DMPEALMal	1.00 ml, 5.96 mmol	0.8730 g, 6.51 mmol	10	crystals **DMPEALMal**
DMPEALMD	1.00 ml, 5.96 mmol	0.9942 g, 6.53 mmol	10	oil
DMPEALTar	1.00 ml, 5.96 mmol	0.9818 g, 6.54 mmol	1	crystals **DMPEALTar**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
DMPEAMale	1.00 ml, 5.96 mmol	0.6957 g, 6.00 mmol	1	crystals **DMPEAMale**
DMPEAMalon	1.00 ml, 5.96 mmol	0.6205 g, 5.96 mmol	1	crystals **DMPEAMalon**
DMPEAMeSO3	1.00 ml, 5.96 mmol	0.82 ml, 5.96 mmol	1	oil
DMPEAoTol	1.00 ml., 5.96 mmol	0.8939 g, 6.57 mmol	10	oil
DMPEAPO4	1.00 ml, 5.96 mmol	0.69 ml, 5.96 mmol	1	poor crystals
DMPEApTol	1.00 ml, 5.96 mmol	0.8996 g, 6.61 mmol	1	amorphous solid
DMPEARMal	1.00 ml. 5.96 mmol	0.8833 g, 6.59 mmol	1	crystals **DMPEARMal**
DMPEARMD	1.00 ml, 5.96 mmol	0.9197 g, 6.04 mmol	1	poor crystals
DMPEARTar	1.00 ml, 5.96 mmol	0.8924 g, 5.95 mmol	5	poor crystals
DMPEASO4	1.00 ml, 5.96 mmol	0.60 ml, 5.96 mmol	1	oil
DMPEASuc	1.00 ml, 5.96 mmol	0.7747 g, 6.56 mmol	1	crystals **DMPEASuc**

Table A.4 Attempted synthesis of phenylpropylammonium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
PPA2CB	1.00 ml, 6.88 mmol	1.2182 g, 7.78 mmol	1	oil
PPA2FB	1.00 ml, 6.88 mmol	1.0856 g, 7.75 mmol	1	amorphous solid
PPA2HB	1.00 ml, 6.88 mmol	1.0673 g, 7.73 mmol	10	oil
PPA3CB	1.00 ml, 6.88 mmol	1.2125 g, 7.74 mmol	1	oil
PPA3FB	1.00 ml, 6.88 mmol	1.0845 g, 7.74 mmol	1	poor crystals
PPA4CB	1.00 ml, 6.88 mmol	1.2125 g, 7.74 mmol	1	poor crystals
PPA4FB	1.00 ml, 6.88 mmol	1.0768 g, 7.68 mmol	1	amorphous solid
PPA4HB	1.00 ml, 6.88 mmol	0.9494 g, 6.87 mmol	2	poor crystals
PPA4HBS	1.00 ml, 6.88 mmol	1.84 ml, 6.88 mmol	2	crystals **PPA4HBS**
PPAAdp	1.00 ml. 6.88 mmol	1.1034 g, 7.55 mmol	1	crystals **PPAAdp**
PPABF4	1.00 ml, 6.88 mmol	1.51 ml, 6.88 mmol	1	liquid
PPABr	1.00 ml, 6.88 mmol	1.16 ml, 6.88 mmol	2	poor crystals
PPABS	1.00 ml, 6.88 mmol	1.0900 g, 6.89 mmol	1	crystals **PPABS**
PPACl	1.00 ml, 6.88 mmol	0.68 ml, 6.88 mmol	5	amorphous solid
PPAClO4	1.00 ml, 6,88 mmol	0.99 ml, 6.88 mmol	1	amorphous solid
PPAEDS	1.00 ml, 6.88 mmol	1.3091 g, 6.88 mmol	3	amorphous solid
PPAEtSO3	1.00 ml, 6.88 mmol	1.08 ml, 6.88 mmol	2	poor crystals
PPAFum	1.00 ml, 6.88 mmol	0.8943 g, 7.70 mmol	1	crystals **PPAFum**
PPAI	1.00 ml, 6.88 mmol	1.71 ml, 6.88 mmol	1	oil
PPALMal	1.00 ml. 6.88 mmol	1.0328 g, 7.70 mmol	1	oil
PPALMD	1.00 ml, 6.88 mmol	1.1711 g, 7.70 mmol	1	crystals **PPALMD**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
PPALTar	1.00 ml, 6.88 mmol	1.1654 g, 7.76 mmol	2	amorphous solid
PPAMale	1.00 ml, 6.88 mmol	0.8019 g, 6.91 mmol	2	crystals **PPAMale**
PPAMalon	1.00 ml, 6.88 mmol	0.7177 g, 6.90 mmol	1	crystals **PPAMalon**
PPAMeSO3	1.00 ml, 6.88 mmol	0.94 ml, 6.88 mmol	1	crystals **PPAMeSO3**
PPAoTol	1.00 ml, 6.88 mmol	1.0595 g, 7.78 mmol	1	amorphous solid
PPAPO4	1.00 ml, 6.88 mmol	0.79 ml, 6.88 mmol	1	oil
PPApTol	1.00 ml, 6.88 mmol	1.0504 g, 7.71 mmol	2	amorphous solid
PPARMal	1.00 ml, 6.88 mmol	1.0391 g, 7.75 mmol	1	oil
PPARMD	1.00 ml, 6.88 mmol	1.0405 g, 6.84 mmol	1	crystals **PPARMD**
PPARTar	1.00 ml, 6.88 mmol	1.0377 g, 6.91 mmol	1	crystals **PPARTar**
PPASO4	1.00 ml, 6.88 mmol	0.71 ml, 6.88 mmol	1	oil
PPASuc	1.00 ml, 6.88 mmol	0.9165 g, 7.76 mmol	1	poor crystals

Table A.5 Attempted synthesis of hydroxyphenethylammonium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
HPEA2CB	0.5044 g, 3.68 mmol	0.6334 g, 4.04 mmol	1	amorphous solid
HPEA2FB	0.5095 g, 3.71 mmol	0.5730 g, 4.09 mmol	1	oil
HPEA2HB	0.5009 g, 3.65 mmol	0.5566 g, 4.03 mmol	1	acid formed
HPEA3CB	0.4990 g, 3.64 mmol	0.6333 g, 4.04 mmol	1	crystals **HPEA3CB**
HPEA3FB	0.5053 g, 3.68 mmol	0.5750 g, 4.10 mmol	1	oil
HPEA4CB	0.5033 g, 3.67 mmol	0.6331 g, 4.04 mmol	1	crystals **HPEA4CB**
HPEA4FB	0.5032 g, 3.67 mmol	0.5687 g, 4.06 mmol	1	poor crystals
HPEA4HB	0.9994 g, 7.29 mmol	1.0076 g, 7.30 mmol	1	crystals **HPEA4HB**
HPEA4HBS	1.0069 g, 7.24 mmol	1.97 ml, 7.34 mmol	2	poor crystals
HPEAAdp	0.5021 g, 3.66 mmol	0.5900 g, 4.04 mmol	1	oil
HPEABF4	1.0060 g, 7.33 mmol	1.61 ml, 7.33 mmol	2	crystals **HPEABF4**
HPEABr	1.0007 g, 7.29 mmol	1.23 ml, 7.29 mmol	1	oil
HPEABS	1.0007 g, 7.29 mmol	1.1574 g, 7.31 mmol	2	amorphous solid
HPEACl	1.0084 g, 7.25 mmol	0.77 ml, 7.35 mmol	1	poor crystals
HPEAClO4	1.0048 g, 7.32 mmol	1.05 ml, 7.32 mmol	1	crystals **HPEAClO4**
HPEAEDS	1.0000 g, 7.29mol	1.3874 g, 7.29 mmol	1	crystals **HPEAEDS**
HPEAEtSO3	1.0077 g, 7.25 mmol	1.16 ml, 7.35 mmol	2	poor crystals
HPEAFum	0.5030 g, 3.67 mmol	0.4726 g, 4.07 mmol	1	poor crystals
HPEAI	0.9962 g, 7.26 mmol	1.86 ml, 8.00 mmol	1	crystals **JAMMAL**[4]
HPEALMal	0.4906 g, 3.58 mmol	0.5298 g, 3.95 mmol	1	oil

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
HPEALMD	0.5047 g, 3.68 mmol	0.6143 g, 4.04 mmol	1	crystals **HPEALMD**
HPEALTar	0.5037 g, 3.67 mmol	0.6076 g, 4.05 mmol	1	crystals **HPEARTar**
HPEAMale	1.0047 g, 7.32 mmol	0.8536 g, 7.35 mmol	1	crystals **HPEAMale**
HPEAMalon	1.0080 g, 7.35 mmol	0.7574 g, 7.28 mmol	1	crystals **HPEAMalon**
HPEAMeSO3	0.9994 g, 7.29 mmol	1.00 ml, 7.29 mmol	2	crystals **HPEAMeSO3**
HPEAoTol	0.4998 g, 3.64 mmol	0.5390 g, 3.96 mmol	1	crystals **HPEAoTol**
HPEAPO4	1.0010 g, 7.30 mmol	0.84 ml, 7.30 mmol	1	crystals **HPEAPO4**
HPEApTol	0.4980 g, 3.63 mmol	0.5442 g, 4.00 mmol	1	crystals **HPEApTol**
HPEARMal	0.4970 g, 3.62 mmol	0.5300 g, 3.95 mmol	1	crystals **HPEARMal**
HPEARMD	1.0035 g, 7.32 mmol	1.1123 g, 7,31 mmol	1	crystals **HPEARMD**
HPEARTar	1.0054 g, 7.33 mmol	1.1057 g, 7.37 mmol	2	poor crystals
HPEASO4	1.0057 g, 7.33 mmol	0.74 ml, 7.33 mmol	2	crystals **HPEASO4**
HPEASuc	0.4910 g, 3.58 mmol	0.4684 g, 3.97 mmol	1	oil

Table A.6 Attempted synthesis of tyrammonium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
TYR2CB	1.0028 g, 7.31 mmol	1.2545 g, 8.01 mmol	1	crystals **TYR2CB**
TYR2FB	1.0197 g, 7.43 mmol	1.1254 g, 8.03 mmol	1	crystals **TYR2FB**
TYR2HB	1.0335 g, 7.53 mmol	1.1386 g, 8.24 mmol	1	acid formed
TYR3CB	1.0161 g, 7.41 mmol	1.2506 g, 7.99 mmol	1	crystals **TYR3CB**
TYR3FB	1.0094 g, 7.36 mmol	1.1250 g, 8.03 mmol	1	crystals **TYR3FB**
TYR4AB	1.0102 g 7.36 mmol	1.1095 g, 8.09 mmol	3	crystals **TYR4AB**
TYR4CB	0.9991 g, 7.28 mmol	1.2449 g, 7.95 mmol	1	crystals **TYR4CB**
TYR4FB	1.0068 g, 7.34 mmol	1.1241 g, 8.02 mmol	1	crystals **TYR4FB**
TYR4HB	1.0025 g, 7.31 mmol	1.0153 g, 7.35 mmol	1	crystals **TYR4HB**
TYR4HBS	1.0097 g, 7.36 mmol	1.97 ml, 7.36 mmol	2	crystals **TYR4HBS**
TYRAdp	1.0065 g, 7.34 mmol	1.1883 g, 8.13 mmol	1	crystals **TYRAdp/TYRAdp2**
TYRBF4	1.0063 g, 7.24 mmol	1.61 ml, 7.34 mmol	1	crystals **TYRBF4**
TYRBr	0.9902 g, 7.22 mmol	1.22 ml, 7.22 mmol	1	crystals **TYRBr**
TYRBS	1.0063 g, 7.34 mmol	1.3046 g, 7.42 mmol	2	crystals **TYRS**
TYRCl	1.0064 g, 7.34 mmol	0.80 ml, 8.07 mmol	1	crystals **TYRAMCL1**[5]
TYRClO4	1.0085 g, 7.34 mmol	1.06 ml, 7.35 mmol	1	crystals **TYRClO4**
TYREDS	1.0059 g, 7.33 mmol	1.4074 g, 7.40 mmol	2	crystals **TYREDS**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
TYREtSO3	1.0010 g, 7.30 mmol	1.15 ml, 7.30 mmol	2	crystals **TYREtSO3**
TYRFum	1.0173 g, 7.41 mmol	0.9409 g, 8.10 mmol	1	crystals **TYRFum**
TYRI	0.9969 g, 7.27 mmol	1.69 ml, 7.27 mmol	1	crystals **TYRI**
TYRLMal	0.9996 g, 7.29 mmol	1.0831 g, 8.08 mmol	1	crystals **TYRLMal**
TYRLMD	1.0235 g, 7.46 mmol	1.2235 g, 8.04 mmol	1	crystals **TYRLMD**
TYRLTar	1.0108 g, 7.37 mmol	1.2466 g, 8.31 mmol	1	crystals **TYRRTar**
TYRMale	1.0018 g, 7.30 mmol	0.8481 g, 7.31 mmol	1	crystals **TYRMale**
TYRMalon	1.0010 g, 7.30 mmol	0.7586 g, 7.29 mmol	2	crystals **TYRMalon**
TYRMeSO3	1.0058 g, 7.33 mmol	1.01 ml, 7.33 mmol	1	crystals **TYRMeSO3**
TYRoTol	1.0007 g, 7.29 mmol	1.1097 g, 8.15 mmol	1	crystals **TYRoTol**
TYRPO4	0.9979 g, 7.27 mmol	0.84 ml, 7.27 mmol	1	crystals **TYRPO4**
TYRpTol	1.0316 g, 7.52 mmol	1.1537 g, 8.47 mmol	1	crystals **TYRpTol**
TYRRMal	1.0051 g, 7.33 mmol	1.0860 g, 8.10 mmol	1	crystals **TYRRMal**
TYRRMD	1.0087 g, 7.35 mmol	1.1194 g, 7.36 mmol	1	crystals **TYRRMD**
TYRRTar	0.9996 g, 7.29 mmol	1.0917 g, 7.27 mmol	1	crystals **TYRRTar**
TYRSO4	1.0038 g, 7.32 mmol	0.83 ml, 8.05 mmol	1	crystals **MDHBUH**[6]
TYRSuc	1.0047 g, 7.32 mmol	0.9572 g, 8.10 mmol	1	crystals **TYRSuc**

Table A.7 Attempted synthesis of α(methylaminomethyl)benzyl alcohol salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
MAMBA2CB	07525 g, 4.98 mmol	0.8622 g, 5.51 mmol	2	amorphous solid
MAMBA2FB	1.0334 g, 6.83 mmol	1.0542 g, 7.52 mmol	1	crystals **MAMBA2FB**
MAMBA2HB	0.7499 g, 4.96 mmol	0.7516 g, 5.44 mmol	10	oil
MAMBA3CB	0.7467 g, 4.94 mmol	0.8677 g, 5.51 mmol	1	crystals **MAMBA3CB**
MAMBA3FB	0.7557 g, 5.00 mmol	0.7701 g, 5.50 mmol	1	amorphous solid
MAMBA4CB	0.7553 g, 5.00 mmol	0.8585 g, 5.48 mmol	3	poor crystals
MAMBA4FB	0.7509 g, 4.97 mmol	0.7642 g, 5.45 mmol	1	crystals **MAMBA4FB**
MAMBA4HB	0.5123 g, 3.39 mmol	0.4353 g, 3.75 mmol	1	crystals **MAMBA4HB**
MAMBA4HBS	1.0245 g, 6.77 mmol	2.00 ml, 7.45 mmol	1	crystals **MAMBA4HBS**
MAMBAAdp	0.7449 g, 4.93 mmol	0.8030 g, 5.49 mmol	1	oil
MAMBABF4	0.2524 g, 1.67 mmol	3.08 ml, 1.84 mmol	1	liquid

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
MAMBABr	1.0165 g, 6.64 mmol	1.25 ml, 7.41 mmol	8	crystals **MAMBABr**
MAMBABS	1.0345 g, 6.84 mmol	1.1901 g, 7.53 mmol	2	crystals **MAMBABS**
MAMBACl	1.0060 g, 6.65 mmol	0.76 ml, 7.29 mmol	1	crystals **MAMBACl**
MAMBAClO4	1.0367 g, 6.86 mmol	1.08 ml 7.55 mmol	1	oil
MAMBAEDS	0.5027 g, 3.32 mmol	0.6998 g, 3.68 mmol	1	crystals **MAMBAEDS**
MAMBAEtSO3	1.0539 g, 6.97 mmol	1.20 ml, 7.63 mmol	1	oil
MAMBAFum	0.7497 g, 4.96 mmol	0.6329 g, 5.45 mmol	2	amorphous solid
MAMBAI	1.0580 g, 7.00 mmol	1.15 ml, 7.67 mmol	1	crystals **MAMBAI**
MAMBALMal	0.7566 g, 5.00 mmol	0.7337 g, 5.47 mmol	2	oil
MAMBALMD	0.7464 g, 4.94 mmol	0.8254 g, 5.42 mmol	1	crystals **MAMBALMD**
MAMBALTar	0.7546 g, 4.99 mmol	0.8185 g, 5.45 mmol	1	oil
MAMBAMale	0.7523 g, 4.97 mmol	0.6346 g, 5.47 mmol		fumaric acid formed
MAMBAMalon	1.0377 g, 6.86 mmol	0.7920 g, 7.61 mmol	1	crystals **MAMBAMalon**
MAMBAMeSO3	1.0382 g, 6.87 mmol	1.05 ml, 7.65 mmol	1	crystals **MAMBAMeSO3**
MAMBAoTol	0.7459 g, 4.93 mmol	0.7348 g, 5.40 mmol	1	poor crystals
MAMBAPO4	1.0373 g, 6.86 mmol	0.88 ml, 7.63 mmol	7	crystals
MAMBApTol	0.7543 g, 4.99 mmol	0.7545 g, 5.54 mmol	3	poor crystals
MAMBARMal	0.7528 g, 4.98 mmol	0.7323 g, 5.46 mmol	10	oil
MAMBARMD	1.0388 g, 6.84 mmol	1.1897 g, 7.82 mmol	1	crystals **MAMBARMD**
MAMBARTar	1.0244 g, 6.77 mmol	1.1201 g, 7.46 mmol	4	oil
MAMBASO4	1.0088, 6.67 mmol	0.76 ml, 7.36 mmol	1	crystals
MAMBASuc	0.7549 g, 4.99 mmol	0.6550 g, 5.55 mmol	1	crystals **MAMBASuc**

Table A.8 Attempted synthesis of ephedrinium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
Epd2AB	1.0200 g, 6.17 mmol	0.9306 g, 6.79 mmol	1	oil
Epd2CB	0.4967 g, 3.01 mmol	0.5159 g, 3.30 mmol	2	crystals **Epd2CB**
Epd2FB	0.4972 g, 3.01 mmol	0.4683 g, 3.34 mmol	1	oil
Epd2HB	0.4971 g, 3.01 mmol	0.4673 g, 3.38 mmol	3	poor crystals
Epd2NB	1.0429 g, 6.31 mmol	1.1694 g, 7.00 mmol	1	crystals **Epd2NB**
Epd3AB	1.0354 g, 6.27 mmol	0.9451 g, 6.89 mmol	1	oil
Epd3CB	0.5082 g, 3.08 mmol	0.5123 g, 3.27 mmol	2	crystals **Epd3CB**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
Epd3FB	0.5011 g 3.03 mmol	0.4708 g, 3.36 mmol	1	oil
Epd3HB	1.0384 g, 6.28 mmol	0.9574 g, 6.93 mmol	1	oil
Epd3NB	1.0384 g, 6.28 mmol	1.1291 g, 6.76 mmol	3	poor crystals
Epd4AB	1.0021, 6.18 mmol	0.9159 g, 6.68 mmol	3	crystals **Epd4AB**
Epd4CB	0.5074 g, 3.07 mmol	0.5118 g, 3.27 mmol	1	crystals **Epd4CB**
Epd4FB	0.5006 g, 3.03 mmol	0.4653 g, 3.35 mmol	1	poor crystals
Epd4HB	0.5024 g, 3.04 mmol	0.4628 g, 3.35 mmol	10	poor crystals
Epd4HBS	0.5052 g, 3.06 mmol	0.90 ml, 3.37 mmol	1	crystals **Epd4HBS**
EPd4NB	1.0265 g, 6.21 mmol	1.1453 g, 6.85 mmol	3	crystals **Epd4NB/Epd4NB2**
EpdAdp	0.5086 g, 3.08 mmol	0.5023 g, 3.44 mmol	1	crystals **GEHJEJ**[7]
EpdBF4	0.4985 g, 3.02 mmol	0.73 ml, 3.32 mmol	1	amorphous solid
EpdBr	0.5062 g, 3.06 mmol	0.57 ml, 3.38 mmol	1	crystals **EpdBr**
EpdBS	0.5038 g, 3.05 mmol	0.5824 g, 3.30 mmol	1	crystals **GEHJIN**[7]
EpdBz	0.5066g 3.07 mmol	0.4119, 3.37 mmol	1	poor crystals
EpdCl	0.5018 g, 3.04 mmol	0.35 ml, 3.34 mmol	1	crystals **EPHECL01**[8]
EpdClO4	0.5066 g, 3.07 mmol	0.48 ml, 3.37 mmol	1	poor crystals
EpdEDS	0.5010 g, 3.03 mmol	0.6327 g, 3.33 mmol	1	crystals **GEHJOT**[7]
EpdEtSO3	0.5034 g, 3.05 mmol	0.53 ml, 3,35 mmol	1	crystals **GEHJUZ**[7]
EpdFum	0.5050 g, 3.06 mmol	0.3954 g, 3.41 mmol	1	amorphous solid
EpdI	0.4999 g, 3.03 mmol	0.77 ml, 3.33 mmol	1	crystals **EpdI**
EpdLMal	0.5091 g, 3.08 mmol	0.4546 g, 3.39 mmol	1	crystals **GEHKEK**[7]
EpdLMD	0.5069 g, 3.07 mmol	0.5199 g, 3.47 mmol	1	crystals **EpdLMD**
EpdLTar	0.5032 g, 3.05 mmol	0.5023 g, 3.35 mmol	1	crystals **GEHLIP**[7]**/GEJMOY**[7]
EpdMale	0.5039 g, 3.05 mmol	0.3958 g, 3.41 mmol	1	crystals **GEHKIO**[7]
EpdMalon	0.5085 g, 3.08 mmol	0.3525 g, 3.39 mmol	1	crystals **GEHKOU**[7]
EpdMeSO3	0.5052 g, 3.06 mmol	0.46 ml, 3.36 mmol	1	crystals **GEHKUA**[7]
EPdmTol	1.0027 g, 6.07 mmol	0.9123 g, 6.70 mmol	1	crystals **EpdmTol**
EpdoTol	0.5072 g, 3.07 mmol	0.4619 g, 3.39 mmol	1	amorphous solid
EpdPO4	0.5062 g, 3.06 mmol	0.39 ml, 3.37 mmol	10	crystals **EPHDHP**[9]**/EPHEDP**[10]
EpdpTol	0.5077 g, 3.07 mmol	0.4665 g, 3.43 mmol	2	poor crystals
EpdRMal	0.5.43 g, 3.05 mmol	0.4497 g, 3.35 mmol	1	oil
EpdRMD	0.5000 g, 3.03 mmol	0.5001 g, 3.29 mmol	1	crystals **EpdRMD**

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
EpdRTar	0.5069 g, 3.07 mmol	0.5150 g, 3.43 mmol	1	poor crystals
EpdSO4	0.5020 g, 3.04 mmol	0.35 ml, 3.34 mmol	1	crystals **EpdSuc**
EpdSuc	0.5072 g, 3.07 mmol	0.3882 g, 3.29 mmol	1	oil

Table A.9 Attempted synthsis of pseudoephedrinium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
PEpd2AB	1.0360 g, 6.27 mmol	0.9552 g, 6.97 mmol	1	crystals **PEpd2AB**
PEpd2CB	0.5040 g, 3.05 mmol	0.5261 g, 3.36 mmol	1	crystals **PEpd2CB**
PEpd2FB	1.0362 g, 6.27 mmol	0.9701 g, 6.92 mmol	1	oil
PEpd2HB	0.4999 g, 3.03 mmol	0.4636 g, 3.36 mmol	1	crystals **PEpd2HB**
PEpd2NB	1.0169 g, 6.15 mmol	1.1290 g, 6.76 mmol	1	crystals **PEpd2NB**
PEpd3AB	1.0212 g, 6.18 mmol	0.9387 g, 6.84 mmol	1	oil
PEpd3CB	0.4973 g, 3.01 mmol	0.5168 g, 3.30 mmol	10	poor crystals
PEpd3FB	1.0284 g, 6.22 mmol	0.9631 g, 6.87 mmol	1	oil
PEpd3HB	1.0248 g, 6.20 mmol	0.9523 g, 6.89 mmol	1	crystals **PEpd3HB**
PEpd3NB	1.3010 g, 7.87 mmol	1.4494 g, 8.67mol	1	oil
PEpd4AB	1.0275 g, 6.22 mmol	0.9338 g, 6.81 mmol	1	crystals **PEpd4AB**
PEpd4CB	0.4993 g, 3.02 mmol	0.5236 g, 3.34 mmol	1	crystals **PEpd4CB**
PEpd4FB	1.0188 g, 6.16 mmol	0.9633 g, 6.80 mmol	1	crystals **PEpd4FB**
PEpd4HB	0.5049 g, 3.06 mmol	0.4683 g, 3.39 mmol	1	amorphous solid
PEpd4HBS	0.5033 g, 3.05 mmol	0.90 ml, 3.36mol	1	crystals **PEpd4HBS**
PEpd4NB	1.0041 g, 6.08 mmol	1.1265 g, 6.74 mmol	1	crystals **PEpd4NB**
PEpdAdp	0.4968 g, 3.01 mmol	0.4782 g, 3.27 mmol	1	crystals **PEpdAdp**
PEpdBF4	0.4975 g, 3.01 mmol	0.73 ml, 3.31 mmol	1	amorphous solid
PEpdBr	0.4950 g, 3.00 mmol	0.56 ml, 3.30 mmol	1	crystals **PEpdBr**
PEpdBS	0.4993 g, 3.02 mmol	0.5610 g, 3.19 mmol	1	crystals **PEpdBS**
PEpdBz	1.0201 g, 6.17 mmol	0.8315 g, 6.81 mmol	1	crystals **PEpdBz**
PEpdCl	0.5031 g, 3.04 mmol	0.33 ml, 3.34 mmol	1	crystals **PEPHCL**[11]

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
PEpdClO4	0.5096 g, 3.08 mmol	0.49 ml, 3.39 mmol	1	crystals **PEpdClO4**
PEpdEDS	0.5048 g, 3.06 mmol	0.6480 g, 3.37 mmol	10	crystals **PEpdEDS**
PEpdEtSO3	0.5058 g, 3.06 mmol	0.53 ml, 3.37 mmol	1	oil
PEpdFum	0.5049 g, 3.06 mmol	0.3952 g, 3.40 mmol	1	amorphous solid
PEpdI	0.5021 g, 3.04 mmol	0.78 ml, 3.34 mmol	1	crystal **PEpdI**
PEpdLMal	0.5073 g, 3.07 mmol	0.4582 g, 3.41 mmol	1	oil
PEpdLMD	0.5071 g, 3.07 mmol	0.5164 g, 3.39 mmol	1	crystals **PEpdLMD**
PEpdLTar	0.5033 g, 3.05 mmol	0.5026 g, 3.35 mmol	1	crystals **PEpdLTar**
PEpdMale	0.5021 g, 3.04 mmol	0.3709 g, 3.20 mmol	1	crystals **PEpdMale**
PEpdMalon	0.5014 g, 3.03 mmol	0.3444 g, 3.31 mmol	10	oil
PEpdMeSO3	0.5043 g, 3.05 mmol	0.46 ml, 3.36 mmol	1	oil
PEpdmTol	1.0195 g, 6.17 mmol	0.9247 g, 6.79 mmol	1	oil
PEpdoTol	0.5036 g, 3.05 mmol	0.4554 g, 3.34 mmol	1	crystals **PEpdoTol**
PEpdPO4	0.5093 g, 3.08 mmol	0.39 ml, 3.39 mmol	10	poor crystals
PEpdpTol	0.5059 g, 3.06 mmol	0.4628 g, 3.40 mmol	1	poor crystals
PEpdRMal	0.5049 g, 3.06 mmol	0.3952 g, 3.40 mmol	1	crystals **PEpdRMal**
PEpdRMD	0.5057 g, 3.06 mmol	0.5143 g, 3.38 mmol	1	amorphous solid
PEpdRTar	0.5001 g, 3.03 mmol	0.4985 g, 3.32 mmol	1	conglomerate
PEpdSO4	0.4964 g, 3.00 mmol	0.34 ml, 3.30 mmol	1	crystals **PEpdSO4**
PEpdSuc	0.4991 g, 3.02 mmol	0.3875 g, 3.28 mmol	10	oil

Table A.10 Attempted synthsis of (-)methylephedrinium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
MEpd2CB	1.0021 g, 5.59 mmol	0.9645 g, 6.16 mmol	2	crystals **MEpd2CB**
MEpd2FB	1.0139 g, 5.66 mmol	0.8606 g, 6.17 mmol	1	crystals **MEpd2FB**
MEpd2HB	1.0046 g, 5.62 mmol	0.8515 g, 6.16 mmol	1	crystals **MEpd2NB**
MEpd3AB	1.0021 g 5.59 mmol	0.8444 g 6.16 mmol	3	crystals **MEpd3FB**
MEpd3CB	1.0072 g, 5.62 mmol	0.9626 g, 6.15 mmol	1	crystals **MEpd3CB**
MEpd3FB	1.0054 g, 5.61 mmol	0.8606 g, 6.14 mmol	1	crystals **MEpd3FB**
MEpd4CB	1.0055 g, 5.61 mmol	0.9631 g, 6.15 mmol	1	crystals **MEpd4CB**
MEpd4FB	1.0001 g, 5.58 mmol	0.8677 g, 6.19 mmol	10	acid formed

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
MEpd4HB	1.0547 g, 5.88 mmol	0.8977 g, 6.50 mmol	4	crystals **MEpd4HB**
MEpd4HBS	1.0927 g, 6.53 mmol	1.93 ml, 7.19 mmol	1	crystals **MEpd4HBS**
MEpdAdp	1.0458 g, 5.83 mmol	0.9381 g, 6.42 mmol	2	crystals **MEpdAdp**
MEpdBF4	0.5054 g, 2.82 mmol	0.68 ml, 3.10 mmol	6	crystals **MEpdBF4**
MEpdBr	0.2546 g, 1.42 mmol	0.28 ml,1.66 mmol	1	crystals **MEpdBr**
MEpdBS	0.4960 g, 2.77 mmol	0.5123 g, 2.91 mmol	1	crystals **MEpdBS**
MEpdCl	0.4995 g, 2.79 mmol	0.30 ml, 3.07 mmol	6	crystals **MEpdCl**
MEpdClO4	0.5042 g, 2.81 mmol	0.41 ml, 2.86 mmol	1	poor crystals
MEpdEDS	0.5095 g, 2.84 mmol	0.5436 g, 2.87 mmol	1	crystals **MEpdEDS**
MEpdEtSO3	1.0362 g, 5.78 mmol	1.00 ml, 6.36 mmol	1	crystals **MEpdEtSO3**
MEpdFum	1,0276 g, 5.73 mmol	0.7155 g, 6.16 mmol	1	acid formed
MEpdI	0.5059 g, 2.82 mmol	0.66 ml, 2.82 mmol	1/9	crystals **MEpdI**
MEpdLMal	1.0063 g, 5.61 mmol	0.8227 g, 6.13 mmol	1	oil
MEpdLMD	0.9843 g, 5.49 mmol	0.9288 g, 6.10 mmol	1	crystals **MEpdLMD**
MEpdLTar	0.9999 g, 5.60 mmol	0.9306 g, 6.20 mmol	1	crystals **MEpdLTar**
MEpdMale	0.2499 g, 1.39 mmol	0.1705 g, 1.47 mmol	1	crystals **MEpdMale**
MEpdMalon	1.0129 g, 5.65 mmol	0.6517 g, 6.26 mmol	1	crystals **MEpdMalon**
MEpdMeSO3	1.0449 g, 5.83 mmol	0.88 ml, 6.41 mmol	1	crystals **MEpdMeSO3**
MEpdoTol	1.0103 g, 5.64 mmol	0.7537 g, 5.54 mmol	2	crystals **MEpdoTol**
MEpdPO4	1.0294 g, 5.74 mmol	075 ml, 6.51 mmol	7	oil
MEpdpTol	1.0063 g, 5.61 mmol	0.7498 g, 5.51 mmol	2	crystals **MEpdpTol**
MEpdRMal	1.0119 g, 5.64 mmol	0.8265 g, 6.16 mmol	10	oil
MEpdRMD	1.0051 g, 5.61 mmol	0.9482 g, 6.23 mmol	1	conglomerate
MEpdRTar	1.0479 g, 5.85 mmol	0.9797 g, 6.53 mmol	4	amorphous solid
MEpdSO4	1.0080 g, 5.62 mmol	0.65 ml, 6.30 mmol	1	crystals **MEpdSO4**
MEpdSuc	1.0235 g, 5.71 mmol	0.7242 g, 6.13 mmol	1	crystals **MEpdSuc**

Table A.11 Attempted synthsis of (+/-)methylephedrinium salts

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
RMEpd2CB	0.9953 g, 5.55 mmol	0.9789 g, 6.25 mmol	1	crystals **RMEpd2CB**
RMEPd2FB	0.9995 g, 5.57 mmol	0.8630 g, 6.16 mmol	1	crystals conglomerate

Salt	Quantity base	Quantity acid	Crystallisation method	Outcome
RMEpd2HB	1.0197 g, 5.69 mmol	0.8426 g, 6.11 mmol	1	acid formed
RMEPd3CB	1.0036 g, 5.60 mmol	0.9611 g, 6.14 mmol	1	crystals **RMEpd3CB**
RMEpd3FB	0.9993 g, 5.57 mmol	0.8613 g, 6.15 mmol	1	crystals **RMEpd3FB**
RMEpd4CB	1.0264 g, 5.72 mmol	0.9810 g, 6.27 mmol	1	crystals conglomerate
RMEpd4FB	1.0054 g, 5.61 mmol	0.8268 g, 5.90 mmol	1	crystals **RMEpd4FB**
RMEpd4HB	1.0299 g, 5.75 mmol	0.8757 g, 6.34 mmol	1	crystals conglomerate
RMEpd4HBS	1.0303 g, 5.75 mmol	1.69 ml, 6.32 mmol	1	crystals **RMEpd4HBS**
RMEpdAdp	0.9997 g, 5.58 mmol	0.9007 g, 6.16 mmol	2	crystals **RMEpdAdp**
RMEpdBF4	0.5010 g, 2.79 mmol	0.67 ml, 3.07 mmol	1	liquid
RMEpdBr	0.9944, 5.55 mmol	1.03 ml, 6.10 mmol	1	crystals **RMEpdBr**
RMEpdBS	1.0140 g, 5.66 mmol	0.9977 g, 6.31 mmol	1	crystals **RMEpdBS**
RMEpdClO4	1.0079 g, 5.62 mmol	0.89 ml, 6.18 mmol	3	crystalline solid
RMEpdEDS	1.0019 g, 5.59 mmol	1.777 g, 6.19 mmol	1	crystals **RMEpdEDS/RMEpdEDS2**
RMEpdEtSO3	1.0007 g, 5.58 mmol	0.893 ml, 6.14 mmol	1	oil
RMEpdFum	1.0072 g, 5.62 mmol	0.7243 g, 6.24 mmol	1	acid formed
RMEpdI	1.0022 g, 5.59 mmol	0.92 ml, 6.15 mmol	1/9	crystals **RMEpdI/RMEpdI2**
RMEpdLMal	1.0052 g, 5.61 mmol	0.8201 g, 6.12 mmol	10	oil
RMEpdLMD	0.7588 g, 4.40 mmol	0.7475 g, 4.91 mmol	2	conglomerate/**RMEpdLMD2**
RMEpdLTar	1.0079 g, 5.62 mmol	0.9202 g, 6.13 mmol	10	amorphous solid
RMEpdMale	1.0018 g, 5.59 mmol	0.7189 g, 6.19 mmol	1	crystals **RMEPdMale**
RMEpdMalon	1.0058 g, 5.61 mmol	0.6451 g, 6.26 mmol	1	crystals **RMEpdMalon**
RMEpdMeSO3	1.0052 g, 5.70 mmol	0.84 ml, 6.12 mmol	1	crystals **RMEpdMeSO3/RMEpdMSO32**
RMEpdoTol	1.0018 g, 5.59 mmol	0.8318 g, 6.11 mmol	1	crystals **RMEpdoTol**
RMEpdPO4	0.9923 g, 5.54 mmol	0.70 ml, 6.09 mmol	1	oil
RMEpdpTol	1.0041 g, 5.60 mmol	0.8369 g, 6.15 mmol	1	crystals conglomerate
RMEpdRMal	0.9970 g, 5.56 mmol	0.8221 g, 6.13 mmol	10	oil
RMEpdRMD	1.0309 g, 5.75 mmol	0.9647 g, 6.24 mmol	1	crystals **RMEpdRMD**
RMEpdRTar	0.9985 g, 5.57 mmol	0.9279 g, 6.18 mmol	1	crystals **RMEpdRTar**
RMEpdSO4	1.0107 g, 5.64 mmol	0.64 ml, 6.20 mmol	1	crystals **RMEpdSO4**
RMEpdSuc	1.0192 g, 5.68 mmol	0.7243 g, 6.18 mmol	2	crystals **RMEpdSuc**

Table A.12 Results from selected salt synthesis The work was carried out by Fabio Pastore using crystallisation method 1.[12]

Base → / Acid ↓	PEA	MPEA	DMPEA	HPEA	TYR	MAMBA	MEpd	RMEpd
Bz	poor crystals	poor crystals	oil	amorphous solid	crystals **TYRBz**	poor crystals	crystals **MEPdBz**	crystals **RMEpdBz**/ conglomerate
2AB	oil	oil	oil	amorphous solid	crystals **TYR2AB**		crystals **MEpd2AB**	crystals **RMEpd2AB**
2NB	amorphous solid	oil	oil	amorphous solid	crystals **TYR2NB**	crystals **MAMBA2NB**	crystals **RMEpd2NB**	crystals **RMEpd2NB**
3AB	oil	oil	oil	oil	oil		crystals **MEpd3AB**	poor crystals
3HB	crystals **PEA3HB**	oil	crystals **DMPEA3HB**	oil	crystals **TYR3HB**		crystals **MEpd3HB**	crystals **RMEpd3HB**
3NB	crystals **PEA3NB**	oil	poor crystals	crystals **HPEA3NB**	crystals **TYR3NB**		oil	crystals **RMEPd3NB**
4AB	crystals **PEA4AB**	oil	poor crystals	crystals **HPEA4AB**	crystals **TYR4AB**		crystals **MEpd4AB**	crystals **RMEpd4AB**
4NB	crystals **PEA4NB**	crystals **MPEA4NB**	crystals **DMPEA4NB**	poor crystals	crystals **TYR4NB**		crystals **MEpd4NB**	crystals **RMEpd4NB**
mTol	crystals **PEAmTol**	oil	oil	oil	crystals **TYRmTol**		oil	crystals **RMEpdmTol**

References

(1) Rademeyer, M. *Acta Crystallographica Section E-Structure Reports Online* **2007**, *63*, O221.

(2) Horn, E.; Tiekink, E. R. T.; Jones, G. P.; Naiola, B. P.; Paleg, L. G. *Acta Crystallographica Section C-Crystal Structure Communications* **1990**, *46*, 1575.

(3) Haynes, D. A.; Pietersen, L. K. *Crystengcomm* **2008**, *10*, 518.

(4) Barlow, R. B.; Johnson, O.; Howard, J. A. K.; Walton, D. C.; Koellner, G. *Acta Crystallographica Section B-Structural Science* **1989**, *45*, 396.

(5) Podder, A.; Dattagupta, J. K.; Saha, N. N.; Saenger, W. *Acta Crystallographica Section B-Structural Science* **1979**, *35*, 649.

(6) Koleva, B. B.; Kolev, T.; Seidel, R. W.; Spiteller, M.; Mayer-Figge, H.; Sheldrick, W. S. *J. Mol. Struct.* **2008**, *888*, 138.
(7) Collier, E. A.; Davey, R. J.; Black, S. N.; Roberts, R. J. *Acta. Cryst.* **2006**, *A62*, 498.
(8) Bergin, R. *Acta Crystallographica Section B-Structural Crystallography and Crystal Chemistry* **1971**, *B 27*, 381.
(9) Hearn, R. A.; Bugg, C. E. *Acta Crystallographica Section B-Structural Science* **1972**, *28*, 3662.
(10) Hearn, R. A.; Freeman, G. R.; Bugg, C. E. *J. Am. Chem. Soc.* **1973**, *95*, 7150.
(11) Mathew, M.; Palenik, G. J. *Acta Crystallographica Section B-Structural Science* **1977**, *33*, 1016.
(12) Duddu, S. P.; Grant, D. J. W. *Pharm. Res.* **1994**, *11*, 1549.

Appendix B - X-ray powder diffraction results

The tables below detail the unit cell parameters derived from the single crystal X-ray diffraction and the X-ray powder data refinements for both the dry and wet powder samples, refer to Section 3.5.2 of Materials and Methods. The dry samples were examined prior to the solubility slurry experiment and the wet samples were examined after the solubility slurry experiment. Where the dry and wet unit cell parameters match those of the single crystal, the measured solubility was deemed to be that of the single crystalline phase and only then was it used in further analysis. Note that as the single crystal unit cells were obtained at low temperature and the powder diffraction cells at room temperature, some disparity between the two is expected.

Table B.1 X-ray powder analysis for phenethylammonium salts

Structure	**Source of unit cell**	**Sp G**	**Cell parameters**						**Goodness of fit (Chi^2)**	**Comment**
			a (Å)	**b (Å)**	**c (Å)**	**α (°)**	**β (°)**	**γ (°)**		
PEA3CB dry	SXD at 123K	$P2_1/n$	14.589	6.294	15.891	90	102.286	90	2.561	
	refined with DASH	$P2_1/n$	14.609	6.299	16.143	90	101.094	90		
PEA3CB wet	refined with DASH	$P2_1/n$	14.450	6.244	15.886	90	102.017	90	4.769	
PEA3FB dry	SXD at 123K	C2/c	30.499	6.818	21.508	90	117.83	90	13.919	
	refined with DASH	C2/c	30.412	6.854	21.774	90	116.531	90		some impurities
PEA3FB wet	refined with DASH	C2/c	30.262	6.891	21.820	90	116.968	90	5.531	
PEA3HB dry	SXD at 123K	P-1	6.058	10.295	10.829	89.160	85.233	88.292	20.418	
	refined with DASH	P-1	6.000	10.364	10.733	89.199	85.774	88.578		some impurities

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
PEA3HB wet	refined with DASH	P-1	5.960	10.253	10.718	88.652	84.463	87.829	11.470	
PEA3NB dry	SXD at 123K	$P2_1/c$	10.685	6.319	21.085	90	92.509	90	2.732	
	refined with DASH	$P2_1/c$	10.622	6.352	21.415	90	92.041	90		
PEA3NB wet	refined with DASH	$P2_1/c$	10.607	6.341	21.379	90	92.081	90	1.908	
PEA4AB dry	SXD at 123K	$P2_12_12_1$	6.267	13.015	16.752	90	90	90	19.031	
	refined with DASH	$P2_12_12_1$	6.301	12.922	16.945	90	90	90		some impurities
PEA4AB wet	refined with DASH	$P2_12_12_1$	6.293	12.937	16.932	90	90	90	3.521	
PEA4FB dry	SXD at 123K	$Pna2_1$	13.492	16.004	6.179	90	90	90	1.928	
	refined with DASH	$Pna2_1$	13.055	17.026	6.277	90	90	90		
PEA4FB wet	refined with DASH	$Pna2_1$	13.492	16.004	6.179	90	90	90	no match	
PEA4HB dry	SXD at 123K	Pc	12.301	13.020	18.357	90	110.201	90	2.043	
	refined with DASH	Pc	12.433	13.049	18.429	90	109.841	90		
PEA4HB wet	refined with DASH	Pc	12.418	13.050	18.416	90	109.789	90	1.711	
PEA4HBS dry	SXD at 123K	$P2_1$	9.905	7.619	10.657	90	113.252	90		
	refined with DASH	$P2_1$	9.990	7.580	10.669	90	112.065	90	5.332	
PEA4HBS wet	refined with DASH	$P2_1$	10.029	7.614	10.707	90	112.117	90	1.601	
PEA4NB dry	SXD at 123K	$P2_1/c$	21.264	6.292	21.201	90	97.735	90	9.553	
	refined with DASH	$P2_1/c$	21.689	6.212	21.254	90	96.943	90		

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
PEA4NB wet	refined with DASH	$P2_1/c$	20.822	6.164	21.132	90	99.590	90	10.308	
PEABF4 dry	SXD at 123K	$P2_1/c$	7.527	36.728	7.396	90	93.149	90	4.939	
	refined with DASH	$P2_1/c$	7.762	36.991	7.593	90	94.466	90		
PEABF4 wet	refined with DASH	$P2_1/c$	7.712	37.010	7.618	90	95.095	90	9.222	
PEABr dry	SXD at 123K	$P2_12_12_1$	4.687	6.142	32.047	90	90	90	3.201	
	refined with DASH	$P2_12_12_1$	32.012	6.144	4.686	90	90	90		
PEABr wet	refined with DASH	$P2_12_12_1$	31.921	6.126	4.673	90	90	90	2.012	
PEACl dry	SXD at 123K	$P2_12_12_1$	4.603	5.906	32.360	90	90	90	3.752	
	refined with DASH	$P2_12_12_1$	4.586	5.884	32.317	90	90	90		
PEACl wet	refined with DASH	$P2_12_12_1$	4.598	5.899	32.309	90	90	90	1.535	
PEAEDS dry	SXD at 123K	C2	7.350	7.239	21.066	90	97.120	90	8.115	
	refined with DASH	C2	7.358	7.295	20.996	90	95.288	90		
PEAEDS wet	refined with DASH	C2	7.355	7.295	20.988	90	95.292	90	6.967	
PEAEtSO3 dry	SXD at 123K	Pbcn	45.789	7.279	7.341	90	90	90	6.329	
	refined with DASH	Pbcn	46.484	7.342	7.435	90	90	90		
PEAEtSO3 wet	refined with DASH	Pbcn	46.235	7.397	7.320	90	90	90	3.260	
PEAFUM dry	SXD at 123K	P-1	9.187	10.574	12.596	81.281	88.918	86.256	5.516	
	refined with DASH	P-1	9.179	10.708	12.605	82.23	89.999	87.514		

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
PEAFum wet	refined with DASH	P-1	9.247	10.745	12.669	81.993	90.149	87.333	7.889	
PEALMD dry	SXD at 123K	$P2_12_12_1$	6.121	7.714	30.616	90	90	90	3.073	
	refined with DASH	$P2_12_12_1$	6.140	7.813	30.933	90	90	90		
PEALMD wet	refined with DASH	$P2_12_12_1$	6.136	7.807	30.939	90	90	90	9.494	
PEAMale dry	SXD at 123K	P-1	12.000	12.878	13.692	62.397	89.363	78.434	4.984	
	refined with DASH	P-1	12.166	13.049	13.940	62.53	89.895	77.500		
PEAMale wet	refined with DASH	P-1	12.086	13.095	14.079	62.402	89.935	78.573	5.161	
PEAMalon dry	SXD at 123K	$P2_1/c$	7.894	8.904	15.907	90	94.015	90	3.690	
	refined with DASH	$P2_1/c$	7.938	8.907	16.076	90	94.854	90		
PEAMalon wey	refined with DASH	$P2_1/c$	7.926	8.905	16.067	90	94.876	90	3.648	
PEAMeSO3 dry	SXD at 123K	C2	7.351	7.204	21.064	90	91.12	90	6.452	
	refined with DASH	C2	7.392	7.231	21.157	90	91.756	90		
PEAMeSO3 wet	refined with DASH	C2	7.391	7.232	21.171	90	91.696	90	1.509	
PEAmTol dry	SXD at 123K	$P2_1/c$	5.968	23.615	14.872	90	92.612	90	no match	
	refined with DASH	$P2_1/c$	5.968	23.615	14.872	90	92.612	90		
PEAmTol wet	refined with DASH	$P2_1/c$	5.968	23.615	14.872	90	92.612	90	no match	
PEApTol dry	SXD at 123K	$P2_1/c$	14.934	6.349	15.915	90	113.165	90	no match	
	refined with DASH	$P2_1/c$	14.934	6.349	15.915	90	113.165	90		

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
PEApTol wet	refined with DASH	$P2_1/c$	14.548	6.327	16.171	90	113.503	90	12.233	some impurities
PEARMal dry	SXD at 123K	P-1	6.058	14.483	15.090	110.974	91.172	95.001	5.128	
	refined with DASH	P-1	6.086	14.456	15.142	111.17	90.092	95.607		
PEARMal wet	refined with DASH	P-1	6.068	14.543	15.179	111.103	89.879	95.785	1.544	
PEARMD dry	SXD at 123K	$P2_1/c$	11.782	20.243	6.002	90	101.549	90	6.147	
	refined with DASH	$P2_1/c$	11.899	20.331	6.010	90	101.433	90		
PEARMD wet	refined with DASH	$P2_1/c$	11.902	20.374	6.002	90	101.317	90	2.177	
PEARTar dry	SXD at 123K	P-1	7.322	7.807	12.602	99.039	96.785	98.517	7.741	
	refined with DASH	P-1	7.315	7.910	12.648	98.901	96.522	98.553		
PEARTar wet	refined with DASH	P-1	7.299	7.898	12.620	98.903	96.441	98.553	2.600	
PEASO4 dry	SXD at 123K	$P2_1/c$	7.607	6.134	23.813	90	94.049	90	6.841	
	refined with DASH	$P2_1/c$	7.781	6.311	24.507	90	93.727	90		
PEASO4 wet	refined with DASH	$P2_1/c$	7.610	6.191	24.113	90	94.495	90	8.454	
PEASuc dry	SXD at 123K	P-1	9.323	10.830	12.703	80.931	86.268	88.868	6.252	
	refined with DASH	P-1	9.370	10.962	12.759	81.833	86.803	89.016		
PEASuc wet	refined with DASH	P-1	9.423	10.947	12.736	81.906	86.723	89.677	8.690	

Table B.2 X-ray powder analysis for methylphenethylaminium salts

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
MPEA2CB dry	SXD at 123K	$Pca2_1$	10.325	17.105	8.543	90	90	90	3.369
	refined with DASH	$Pca2_1$	10.305	17.355	8.634	90	90	90	
MPEA2CB wet	refined with DASH	$Pca2_1$	10.321	17.384	8.647	90	90	90	2.493
MPEA2HB dry	SXD at 123K	C2/c	16.003	7.589	24.662	90	93.733	90	7.216
	refined with DASH	C2/c	16.271	7.503	25.133	90	94.098	90	
MPEA2HB wet	refined with DASH	C2/c	16.385	7.482	25.202	90	94.014	90	10.299
MPEA4HB dry	SXD at 123K	$P2_1/a$	9.919	9.708	15.773	90	98.202	90	5.395
	refined with DASH	$P2_1/a$	9.930	9.790	15.798	90	97.301	90	
MPEA4HB wet	refined with DASH	$P2_1/a$	9.944	9.811	15.822	90	97.349	90	3.025
MPEA4HBS dry	SXD at 123K	$P2_12_12_1$	6.352	14.079	17.918	90	90	90	4.573
	refined with DASH	$P2_12_12_1$	6.426	13.924	18.240	90	90	90	
MPEA4HBS wet	refined with DASH	$P2_12_12_1$	6.424	13.917	18.231	90	90	90	3.327
MPEA4NB dry	SXD at 123K	P-1	13.150	16.502	31.208	78.781	84.108	68.482	13.915
	refined with DASH	P-1	13.160	16.626	30.945	78.210	84.469	68.083	
MPEA4NB wet	refined with DASH	P-1	13.160	16.626	30.945	78.210	84.469	68.083	2.749
MPEAAdp dry	SXD at 123K	C2/c	26.982	6.136	22.915	90	126.395	90	no match
	refined with DASH	C2/c	26.982	6.136	22.915	90	126.395	90	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
MPEAAdp wet	refined with DASH	C2/c	26.982	6.136	22.915	90	126.395	90	no match
MPEAEDS dry	SXD at 123K	$P2_1/c$	5.472	18.438	16.940	90	90.536	90	no match
	refined with DASH	$P2_1/c$	5.472	18.438	16.940	90	90.536	90	
MPEAEDS wet	refined with DASH	$P2_1/c$	5.472	18.438	16.940	90	90.536	90	no match
MPEALMal dry	SXD at 123K	$P2_1$	6.326	8.315	13.162	90	100.395	90	
	refined with DASH	$P2_1$	6.375	8.372	13.329	90	100.447	90	3.194
MPEALMal wet	refined with DASH	$P2_1$	6.359	8.349	13.298	90	100.468	90	1.247
MPEALTar dry	SXD at 123K	$P2_1$	7.687	6.813	13.861	90	91.219	90	8.64
	refined with DASH	$P2_1$	7.708	6.854	13.892	90	91.182	90	
MPEALTar wet	refined with DASH	$P2_1$	7.707	6.858	13.896	90	91.167	90	1.869
MPEAMale dry	SXD at 123K	C2/c	37.403	9.534	33.256	90	117.914	90	no match
	refined with DASH	C2/c	37.403	9.534	33.256	90	117.914	90	
MPEAMale wet	refined with DASH	C2/c	37.531	9.624	33.407	90	118.266	90	15.416
MPEAPO4 dry	SXD at 123K	Pcab	8.157	11.076	25.967	90	90	90	no match
	refined with DASH	Pcab	8.157	11.076	25.967	90	90	90	
MPEAPO4 wet	refined with DASH	Pcab	8.207	11.110	26.053	90	90	90	2.151
MPEARMD dry	SXD at 123K	$P2_1/c$	5.919	33.077	7.842	90	93.140	90	no match
	refined with DASH	$P2_1/c$	5.919	33.077	7.842	90	93.140	90	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
MPEARMD wet	refined with DASH	$P2_1/c$	5.919	33.077	7.842	90	93.140	90	no match

Table B.3 X-ray powder analysis for dimethylphenethylaminium salts

Structure	Source of unit cell	Sp G	Cell Parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
DMPEA2HB dry	SXD at 123K	P-1	9.631	10.392	15.555	99.184	92.714	90.846	7.729	
	Refined with DASH	P-1	9.632	10.399	15.498	101.064	91.980	90.628		
DMPEA2HB wet	Refined with DASH	P-1	9.853	10.571	15.978	99.969	92.453	89.888	3.707	
DMPEA3HB dry	SXD at 123K	$P2_1/n$	9.022	8.077	21.708	90	99.568	90		
	Refined with DASH	$P2_1/n$	9.022	8.077	21.708	90	99.568	90	no match	
DMPEA3HB wet	Refined with DASH	$P2_1/n$	9.022	8.077	21.708	90	99.568	90	no match	
DMPEA4HB dry	SXD at 123K	$P2_12_12_1$	6.123	15.608	15.985	90	90	90	10.486	
	Refined with DASH	$P2_12_12_1$	6.221	15.758	15.862	90	90	90		
DMPEA4HB wet	Refined with DASH	$P2_12_12_1$	6.233	15.829	15.885	90	90	90	5.192	
DMPEA4NB dry	SXD at 123K	P-1	6.853	11.486	16.062	77.840	85.201	84.643	no match	
	Refined with DASH	P-1	6.853	11.486	16.062	77.840	85.201	84.643		
DMPEA4NB wet	Refined with DASH	P-1	6.853	11.486	16.062	77.840	85.201	84.643	no match	
DMPEAAdp dry	SXD at 123K	C2/c	23.356	5.523	27.531	90	115.824	90	11.871	

Structure	Source of unit cell	Sp G	Cell Parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	Refined with DASH	C2/c	22.381	5.374	27.046	90	79.422	90		some impurities
DMPEAAdp wet	Refined with DASH	C2/c	23.356	5.523	27.531	90	115.824	90	no match	
DMPEABS dry	SXD at 123K	$P2_1/c$	18.501	7.387	12.283	90	96.669	90	6.751	
	Refined with DASH	$P2_1/c$	18.592	7.455	12.369	90	97.29	90		
DMPEABS wet	Refined with DASH	$P2_1/c$	18.631	7.474	12.392	90	97.269	90	1.833	
DMPEAClO4 dry	SXD at 123K	P-1	5.910	14.678	14.735	67.016	87.92	79.466	15.222	
	Refined with DASH	P-1	5.902	14.533	14.642	67.689	88.018	79.364		some impurities
DMPEAClO4 wet	Refined with DASH	P-1	5.862	14.457	14.763	67.012	87.393	78.544	7.065	
DMPEALTar dry	SXD at 123K	P1	7.141	7.189	8.779	72.322	79.655	81.047	15.085	
	Refined with DASH	P1	7.118	7.228	8.844	72.609	79.367	80.942		some impurities
DMPEALTar wet	Refined with DASH	P1	7.138	7.241	8.862	72.63	79.387	80.966	1.463	
DMPEAMalon dry	SXD at 123K	$P2_1/c$	7.327	6.207	29.201	90	93.046	90	no match	
	Refined with DASH	$P2_1/c$	7.327	6.207	29.201	90	93.046	90		
DMPEAMalon wet	Refined with DASH	$P2_1/c$	7.521	6.243	29.237	90	93.234	90	1.663	
DMPEARMal dry	SXD at 123K	P-1	10.929	11.420	13.100	71.630	86.473	72.392	10.401	
	Refined with DASH	P-1	11.040	11.346	13.468	71.742	85.781	71.355		
DMPEARMal wet	Refined with DASH	P-1	11.068	11.401	13.482	71.926	85.996	71.191	3.052	
DMPEASuc dry	SXD at 123K	$P2_1/c$	9.032	6.470	24.070	90	93.363	90	4.803	

Structure	Source of unit cell	Sp G	Cell Parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	Refined with DASH	$P2_1/c$	8.956	6.535	24.237	90	92.879	90		
DMPEASuc wet	Refined with DASH	$P2_1/c$	9.032	6.470	24.070	90	93.363	90	no match	

Table B.4 X-ray powder analysis for phenylpropylammonium salts

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
PPA4HBS dry	SXD at 123K	$P2_1/n$	5.737	19.924	13.468	90	100.714	90	8.964	
	refined with DASH	$P2_1/n$	5.807	20.170	13.575	90	102.851	90		
PPA4HBS wet	refined with DASH	$P2_1/n$	5.815	20.216	13.574	90	102.834	90	1.853	
PPAAdp dry	SXD at 123K	P-1	6.175	11.783	11.971	62.833	85.136	80.020	4.506	
	refined with DASH	P-1	6.208	11.760	12.193	62.948	84.614	79.596		
PPAAdp wet	refined with DASH	P-1	6.215	11.765	12.197	62.938	84.655	798.584	4.325	
PPABS dry	SXD at 123K	Pbca	8.514	22.158	31.100	90	90	90	29.973	
	refined with DASH	Pbca	8.445	21.946	31.098	90	90	90		some impurities
PPABS wet	refined with DASH	Pbca	8.431	21.878	30.917	90	90	90	8.414	
PPAFum dry	SXD at 123K	$P2_1/c$	9.410	10.920	25.239	90	91.882	90	9.736	
	refined with DASH	$P2_1/c$	9.424	10.954	25.354	90	91.218	90		
PPAFum wet	refined with DASH	$P2_1/c$	9.443	10.971	25.410	90	91.179	90	6.737	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
PPALMD dry	SXD at 123K	$P2_1$	11.056	6.225	11.345	90	96.309	90	no match	
	refined with DASH	$P2_1$	11.056	6.225	11.345	90	96.309	90		
PPALMD wet	refined with DASH	$P2_1$	11.056	6.225	11.345	90	96.309	90	no match	
PPAMale dry	SXD at 123K	C2/c	28.669	5.619	18.070	90	111.282	90	8.869	
	refined with DASH	C2/c	28.866	5.643	18.163	90	111.077	90		
PPAMale wet	refined with DASH	C2/c	28.839	5.642	18.149	90	111.120	90	2.493	
PPAMalon dry	SXD at 123K	$P2_1/c$	8.120	19.937	14.791	90	91.621	90		
	refined with DASH	$P2_1/c$	8.151	20.133	14.828	90	91.104	90	10.041	
PPAMalon wet	refined with DASH	$P2_1/c$	8.137	20.010	14.828	90	91.119	90	6.204	
PPAMeSO3 dry	SXD at 123K	$Pna2_1$	8.933	24.264	5.273	90	90	90		
	refined with DASH	$Pna2_1$	9.001	24.622	5.322	90	90	90	5.600	
PPAMeSO3 wet	refined with DASH	$Pna2_1$	8.933	24.264	5.273	90	90	90	no match	
PPARMD dry	SXD at 123K	P-1	5.760	9.294	14.786	100.018	96.093	96.636	33.547	
	refined with DASH	P-1	5.710	9.242	14.672	100.176	96.675	96.967		some impurities
PPARMD wet	refined with DASH	P-1	5.703	9.266	14.709	100.291	96.730	97.155	24.808	some impurities
PPARTar dry	SXD at 123K	P-1	7.171	8.658	12.698	98.085	105.273	95.863	10.895	
	refined with DASH	P-1	7.176	8.727	12.772	97.869	105.007	95.931		
PPARTar wet	refined with DASH	P-1	7.182	8.735	12.776	97.901	104.991	95.977	4.256	

Table B.5 X-ray powder analysis for hydroxyphenethylammonium salts

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
HPEA3CB dry	SXD at 123K	$P2_1/c$	15.890	7.634	11.784	90	95.419	90	2.725	
	refined by DASH	$P2_1/c$	15.935	7.718	11.877	90	95.637	90		
HPEA3CB wet	refined by DASH	$P2_1/c$	15.915	7.708	11.862	90	95.616	90	2.788	
HPEA3NB dry	SXD at 123K	$P2_1/c$	14.504	8.216	17.630	90	94.735	90	20.632	
	refined by DASH	$P2_1/c$	14.626	8.245	17.629	90	93.937	90		some impurities
HPEA3NB wet	refined by DASH	$P2_1/c$	14.504	8.216	17.630	90	94.735	90	no match	
HPEA4AB dry	SXD at 123K	$P2_12_12_1$	5.678	14.078	17.315	90	90	90	14.748	
	refined by DASH	$P2_12_12_1$	5.706	14.076	17.534	90	90	90		some impurities
HPEA4AB wet	refined by DASH	$P2_12_12_1$	5.694	14.076	17.444	90	90	90	6.34	
HPEA4CB dry	SXD at 123K	Pcab	7.212	12.3977	33.356	90	90	90	1.916	
	refined by DASH	Pcab	7.401	12.449	33.557	90	90	90		
HPEA4CB wet	refined by DASH	Pcab	7.401	12.448	33.558	90	90	90	1.709	
HPEA4HB dry	SXD at 123K	$P2_1nb$	6.184	12.344	18.827	90	90	90	16.34	
	refined by DASH	$P2_1nb$	6.202	12.507	18.822	90	90	90		some impurities
HPEA4HB wet	refined by DASH	$P2_1nb$	6.184	12.5	18.769	90	90	90	8.811	
HPEAEDS dry	SXD at 123K	P-1	9.064	10.766	11.560	94.931	100.011	109.009	15.204	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined by DASH	P-1	9.067	10.792	11.372	95.93	98.781	109.17		some impurities
HPEAEDS wet	refined by DASH	P-1	9.193	10.872	11.538	95.096	99.713	109.752	1.316	
HPEALMD dry	SXD at 123K	$P2_12_12_1$	8.784	11.916	28.457	90	90	90	6.012	
	refined by DASH	$P2_12_12_1$	8.798	11.967	28.767	90	90	90		
HPEALMD wet	refined by DASH	$P2_12_12_1$	8.806	11.994	28.788	90	90	90	1.864	
HPEAoTol dry	SXD at 123K	$P2_1/n$	9.089	5.996	28.941	90	90.093	90	2.077	
	refined by DASH	$P2_1/n$	9.116	6.01	29.391	90	90.848	90		
HPEAoTol wet	refined by DASH	$P2_1/n$	9.115	6.011	29.393	90	90.861	90	4.575	
HPEAPO4 dry	SXD at 123K	$P2_1/c$	7.769	27.346	11.449	90	94.873	90	no match	
	refined by DASH	$P2_1/c$	7.769	27.346	11.449	90	94.873	90		
HPEAPO4 wet	refined by DASH	$P2_1/c$	7.769	27.346	11.449	90	94.873	90	no match	
HPEApTol dry	SXD at 123K	Pcab	7.368	12.413	33.799	90	90	90	no match	
	refined by DASH	Pcab	7.368	12.413	33.799	90	90	90		
HPEApTol wet	refined by DASH	Pcab	7.368	12.413	33.799	90	90	90	no match	
HPEARMD dry	SXD at 123K	Pcab	11.718	9.114	27.782	90	90	90	4.968	
	refined by DASH	Pcab	11.783	9.053	28.213	90	90	90		
HPEARMD wet	refined by DASH	Pcab	11.718	9.114	27.782	90	90	90	no match	

Table B.6 X-ray powder analysis for tyrammonium salts

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
TYR2AB dry	SXD at 123	$P2_1/c$	10.809	7.768	16.341	90	93.829	90	9.877	
	refined with DASH	$P2_1/c$	10.799	7.756	16.463	90	93.723	90		
TYR2AB wet	refined with DASH	$P2_1/c$	10.824	7.775	16.496	90	93.726	90	1.116	
TYR2CB dry	SXD at 123	$P2_1/c$	11.254	12.428	11.617	90	116.306	90	5.834	
	refined with DASH	$P2_1/c$	11.394	12.346	11.731	90	116.764	90		
TYR2CB wet	refined with DASH	$P2_1/c$	11.370	12.332	11.697	90	116.825	90	2.59	
TYR2FB dry	SXD at 123	$P2_1$	10.982	12.205	10.996	90	111.243	90	3.35	
	refined with DASH	$P2_1$	11.023	12.179	11.073	90	111.581	90		
TYR2FB wet	refined with DASH	$P2_1$	11.007	12.165	11.060	90	111.596	90	2.456	
TYR3CB dry	SXD at 123	C2/c	24.856	8.101	19.464	90	133.43	90	6.836	
	refined with DASH	C2/c	24.758	8.117	19.787	90	133.554	90		
TYR3CB wet	refined with DASH	C2/c	24.706	8.102	19.763	90	133.567	90	2.013	
TYR3FB dry	SXD at 123	$P2_1/c$	11.490	11.439	10.861	90	107.525	90	11.991	
	refined with DASH	$P2_1/c$	11.406	11.557	10.853	90	107.157	90		some impurities
TYR3FB wet	refined with DASH	$P2_1/c$	11.429	11.567	10.864	90	107.173	90	6.456	
TYR3HB dry	SXD at 123	P-1	8.159	8.719	10.639	85.706	76.200	63.787	3.593	
	refined with DASH	P-1	8.128	8.740	10.724	86.340	75.850	64.210		

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
TYR3HB wet	refined with DASH	P-1	8.121	8.730	10.705	86.339	75.866	64.190	2.233	
TYR3NB dry	SXD at 123	$P2_1/c$	10.494	11.592	12.089	90	93.465	90	4.126	
	refined with DASH	$P2_1/c$	10.350	11.670	12.225	90	93.683	90		
TYR3NB wet	refined with DASH	$P2_1/c$	10.392	11.699	12.260	90	93.608	90	2.307	
TYR4AB dry	SXD at 123	$P2_1/c$	11.508	11.284	10.903	90	107.037	90		
	refined with DASH	$P2_1/c$	11.522	11.343	10.969	90	107.450	90	23.887	some impurities
TYR4AB wet	refined with DASH	$P2_1/c$	11.508	11.284	10.903	90	107.037	90	no match	
TYR4CB dry	SXD at 123	P-1	15.857	17.599	22.088	105.676	96.763	99.335	no match	
	refined with DASH	P-1	15.857	17.599	22.088	105.676	96.763	99.335		
TYR4CB wet	refined with DASH	P-1	15.857	17.599	22.088	105.676	96.763	99.335	no match	
TYR4FB dry	SXD at 123	$P2_1/c$	11.999	11.332	10.754	90	109.754	90	4.513	
	refined with DASH	$P2_1/c$	11.919	11.439	10.881	90	109.232	90		
TYR4FB wet	refined with DASH	$P2_1/c$	11.849	11.410	10.848	90	109.298	90	5.004	
TYR4HB dry	SXD at 123	P-1	9.975	15.162	18.641	76.3	86.480	84.892	8.454	
	refined with DASH	P-1	10.002	15.286	18.797	76.422	86.605	85.123		
TYR4HB wet	refined with DASH	P-1	9.971	15.236	18.644	76.561	86.285	84.936	2.476	
TYR4HBS dry	SXD at 123	$P2_12_12_1$	7.626	34.974	10.916	90	90	90	2.015	
	refined with DASH	$P2_12_12_1$	7.691	34.984	10.992	90	90	90		

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
TYR4HBS wet	refined with DASH	$P2_12_12_1$	7.657	34.808	10.959	90	90	90	1.406	
TYR4NB dry	SXD at 123	$P2_1/c$	7.080	6.178	67.751	90	92.518	90	10.35	
	refined with DASH	$P2_1/c$	7.102	6.163	67.629	90	91.404	90		
TYR4NB wet	refined with DASH	$P2_1/c$	7.080	6.178	67.751	90	92.518	90	no match	
TYRAdp TYRAdp2 dry	SXD at 123	$P2_1/c$	21.110	5.962	24.603	90	105.911	90	8.447	
	SXD at 123	$P2_1/n$	8.625	15.190	8.759	90	93.826	90		
	refined with DASH	$P2_1/c$	21.155	6.040	24.460	90	106.513	90		
TYRApd wet	refined with DASH	$P2_1/n$	8.551	14.983	8.790	90	95.076	90	11.799	fits TYRAdp2
TYRBF4 dry	SXD at 123	Pbca	11.998	7.229	24.615	90	90	90	no match	
	refined with DASH	Pbca	11.998	7.229	24.615	90	90	90		
TYRBF4 wet	refined with DASH	Pbca	11.852	7.343	24.732	90	90	90	1.852	
TYRBr dry	SXD at 123	Pbcn	20.143	10.969	8.275	90	90	90	3.498	
	refined with DASH	Pbcn	20.126	11.002	8.391	90	90	90		
TYRBr wet	refined with DASH	Pbcn	20.107	10.992	8.377	90	90	90	2.565	
TYRBz dry	SXD at 123	$P2_1$	10.869	12.028	11.085	90	110.752	90	3.384	
	refined with DASH	$P2_1$	10.899	11.692	11.452	90	111.591	90		
TYRBz wet	refined with DASH	$P2_1$	10.919	11.716	11.482	90	111.571	90	1.439	
TYRCl dry	SXD at 123	Pbcn	19.973	10.768	8.246	90	90	90	4.705	

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	Pbcn	19.917	10.735	8.231	90	90	90		
TYRCl wet	refined with DASH	Pbcn	19.921	10.740	8.231	90	90	90	1.467	
TYRClO4 dry	SXD at 123	$P2_1/c$	7.394	25.122	11.685	90	90.896	90	1.608	
	refined with DASH	$P2_1/c$	7.394	25.240	11.722	90	90.257	90		
TYRClO4 wet	refined with DASH	$P2_1/c$	7.371	25.092	11.698	90	91.866	90	1.709	
TYREDS dry	SXD at 123	Pbca	9.561	9.554	22.777	90	90	90	6.648	
	refined with DASH	Pbca	9.575	9.671	22.916	90	90	90		
TYREDS wet	refined with DASH	Pbca	9.562	9.666	22.894	90	90	90	1.62	
TYREtSO3 dry	SXD at 123	$P2_1/c$	10.445	20.679	10.837	90	91.198	90	3.569	
	refined with DASH	$P2_1/c$	10.434	20.798	10.923	90	91.421	90		
TYREtSO3 wet	refined with DASH	$P2_1/c$	10.384	21.161	10.844	90	92.148	90	2.236	
TYRFum dry	SXD at 123	P-1	8.878	8.977	9.469	116.911	97.833	91.099	8.963	
	refined with DASH	P-1	8.884	8.980	9.577	116.857	98.093	92.055		
TYRFum wet	refined with DASH	P-1	8.890	8.979	9.576	116.85	98.132	92.013	1.707	
TYRLMal dry	SXD at 123	$P2_1$	11.891	7.796	11.955	90	100.160	90		
	refined with DASH	$P2_1$	11.891	7.796	11.955	90	100.160	90	no match	
TYRLMal wet	refined with DASH	$P2_1$	11.899	7.903	11.967	90	100.700	90	1.797	
TYRLMD dry	SXD at 123	$P2_1$	8.911	8.363	9.658	90	91.246	90	2.369	

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	$P2_1$	8.920	8.415	9.660	90	91.571	90		
TYRLMD wet	refined with DASH	$P2_1$	8.921	8.416	9.662	90	91.563	90	1.64	
TYRLTar dry	SXD at 123	$P2_1$	11.690	7.760	12.324	90	100.013	90	no match	
	refined with DASH	$P2_1$	11.690	7.760	12.324	90	100.013	90		
TYRLTar wet	refined with DASH	$P2_1$	11.690	7.760	12.324	90	100.013	90	no match	
TYRMale dry	SXD at 123	$P2_1/c$	7.692	5.686	27.938	90	103.047	90	2.959	
	refined with DASH	$P2_1/n$	7.738	5.708	27.512	90	93.660	90		
TYRMale wet	refined with DASH	$P2_1/n$	7.735	5.704	27.491	90	93.692	90	1.668	
TYRMalon dry	SXD at 123	$P2_1/c$	13.303	7.861	11.344	90	106.174	90	no match	
	refined with DASH	$P2_1/c$	13.303	7.861	11.344	90	106.174	90		
TYRMalon wet	refined with DASH	$P2_1/c$	13.303	7.861	11.344	90	106.174	90	no match	
TYRMeSO3 dry	SXD at 123	$P2_12_12_1$	5.026	10.074	21.713	90	90	90	6.696	
	refined with DASH	$P2_12_12_1$	5.100	10.106	21.653	90	90	90		
TYRMeSO3 wet	refined with DASH	$P2_12_12_1$	5.094	10.099	21.617	90	90	90	1.548	
TYRmTol dry	SXD at 123	$P2_1/c$	12.864	18.489	12.594	90	97.301	90	7.656	
	refined with DASH	$P2_1/c$	13.165	18.628	12.757	90	101.929	90		
TYRmTol wet	refined with DASH	$P2_1/c$	13.159	18.665	12.628	90	101.987	90	7.205	
TYRoTol dry	SXD at 123	$P2_1/c$	11.453	12.250	11.622	90	116.74	90	2.598	

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	$P2_1/c$	11.556	12.219	11.785	90	117.183	90		
TYRoTol wet	refined with DASH	$P2_1/c$	11.571	12.211	11.787	90	117.186	90	4.843	
TYRpTol dry	SXD at 123	$P2_1/c$	11.480	11.360	11.050	90	104.932	90	8.212	
	refined with DASH	$P2_1/c$	11.466	11.441	11.129	90	105.634	90		
TYRpTol wet	refined with DASH	$P2_1/c$	11.460	11.442	11.127	90	105.641	90	3.007	
TYRRMal dry	SXD at 123	$Pna2_1$	7.636	30.036	6.279	90	90	90	6.039	
	refined with DASH	$Pna2_1$	7.608	30.129	6.312	90	90	90		
TYRRMal wet	refined with DASH	$Pna2_1$	7.598	30.093	6.312	90	90	90	2.544	
TYRRMD dry	SXD at 123	P-1	6.445	10.114	12.213	91.239	99.455	96.794		
	refined with DASH	P-1	6.445	10.114	12.213	91.239	99.455	96.794	no match	
TYRRMD wet	refined with DASH	P-1	6.445	10.114	12.213	91.239	99.455	96.794	no match	
TYRRTar dry	SXD at 123	P-1	7.265	7.948	12.585	77.231	85.330	79.854	4.811	
	refined with DASH	P-1	7.257	8.055	12.521	77.826	85.518	80.057		
TYRRTar wet	refined with DASH	P-1	7.245	8.040	12.496	77.833	85.536	80.077	2.739	
TYRSO4 dry	SXD at 123	$P2_1/c$	7.165	22.819	11.729	90	98.274	90	no match	
	refined with DASH	$P2_1/c$	7.165	22.819	11.729	90	98.274	90		
TYRSO4 wet	refined with DASH	$P2_1/c$	7.345	23.377	11.888	90	98.189	90	6.579	
TYRSuc dry	SXD at 123	$P2_1/c$	11.494	7.550	12.515	90	99.865	90	5.173	

Structure	Source of cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	$P2_1/c$	11.551	7.587	12.482	90	100.323	90		
TYRSuc wet	refined with DASH	$P2_1/c$	11.495	7.550	12.425	90	100.33	90	4.156	

|**Table B.7** X-ray powder analysis of α(methylaminomethyl)benzyl alcohol salts

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MAMBA2FB dry	SXD at 123K	$P2_1/c$	5.830	22.515	11.368	90	95.087	90	2.05	
	refined with DASH	$P2_1/c$	5.840	22.736	11.630	90	94.917	90		
MAMBA2FB wet	refined with DASH	$P2_1/c$	5.862	22.813	11.668	90	94.924	90	1.326	
MAMBA2NB dry	SXD at 123K	$P2_12_12_1$	5.983	12.340	20.897	90	90	90	7.033	
	refined with DASH	$P2_12_12_1$	6.013	12.391	21.176	90	90	90		
MAMBA2NB wet	refined with DASH	$P2_12_12_1$	6.007	12.382	21.163	90	90	90	2.782	
MAMBA3CB dry	SXD at 123K	$P2_1/c$	6.019	11.235	22.256	90	94.767	90	2.873	
	refined with DASH	$P2_1/c$	6.092	11.459	22.344	90	94.755	90		
MAMBA3CB wet	refined with DASH	$P2_1/c$	6.067	11.422	22.261	90	94.750	90	2.258	
MAMBA4FB dry	SXD at 123K	$P2_1/c$	11.899	8.343	33.004	90	103.093	90	3.722	
	refined with DASH	$P2_1/c$	11.780	8.361	32.717	90	102.448	90		
MAMBA4FB wet	refined with DASH	$P2_1/c$	11.899	8.343	33.004	90	103.093	90	no match	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MAMBA4HB dry	SXD at 123K	$P2_1/c$	15.621	9.654	10.222	90	99.898	90	2.032	
	refined with DASH	$P2_1/c$	15.776	9.671	10.234	90	100.258	90		
MAMBA4HB wet	refined with DASH	$P2_1/c$	15.807	9.694	10.250	90	100.419	90	2.898	
MAMBA4HBS dry	SXD at 123K	C2/c	30.012	6.030	23.013	90	131.923	90		
	refined with DASH	C2/c	30.433	6.075	23.164	90	132.302	90	2.053	
MAMBA4HBS wet	refined with DASH	C2/c	30.471	6.088	23.196	90	132.307	90	1.624	fits MAMBA4HBS2
MAMBABr dry	SXD at 123K	$P2_1/c$	12.792	6.972	12.219	90	110.301	90	2.196	
	refined with DASH	$P2_1/c$	12.931	6.996	12.402	90	111.435	90		
MAMBABr wet	refined with DASH	$P2_1/c$	12.988	7.023	12.519	90	111.664	90	2.673	
MAMBAEDS dry	SXD at 123K	P-1	5.451	9.122	17.026	96.474	90.868	93.155		
	refined with DASH	P-1	5.470	9.176	17.175	97.085	90.780	93.036	9.360	
MAMBAEDS wet	refined with DASH	P-1	5.451	9.122	17.026	96.474	90.868	93.155	no match	
MAMBAI dry	SXD at 123K	$P2_1/c$	13.971	5.731	14.807	90	115.219	90	1.265	
	refined with DASH	$P2_1/c$	13.977	5.778	14.925	90	115.549	90		
MAMBAI wet	refined with DASH	$P2_1/c$	13.971	5.731	14.807	90	115.219	90	no match	
MAMBALMD dry	SXD at 123K	C2	19.229	5.699	18.232	90	125.023	90	5.001	
	refined with DASH	C2	19.185	5.714	18.240	90	124.371	90		
MAMBALMD wet	refined with DASH	C2	19.235	5.740	18.265	90	124.345	90	1.623	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MAMBAMalon dry	SXD at 123K	$P2_1/a$	7.443	33.542	10.263	90	90.105	90	2.526	
	refined with DASH	$P2_1/a$	7.477	33.228	10.223	90	90.295	90		
MAMBAMalon wet	refined with DASH	$P2_1/a$	7.513	33.463	10.268	90	90.273	90	1.83	
MAMBASuc dry	SXD at 123K	$Pca2_1$	24.998	5.930	8.984	90	90	90	3.321	
	refined with DASH	$Pca2_1$	25.303	5.907	8.990	90	90	90		
MAMBASuc wet	refined with DASH	$Pca2_1$	25.298	5.909	8.995	90	90	90	1.704	

Table B.8 X-ray powder analysis for (-)ephedrinium salts

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
Epd dry	SXD at 123K	$C222_1$	7.364	11.255	24.144	90	90	90	12.157	
	refined with DASH	$C222_1$	7.403	11.335	24.303	90	90	90		almost right fit
Epd wet	refined with DASH	$C222_1$	7.412	11.352	24.344	90	90	90	3.122	fits Epd2
EPd2CB dry	SXD at 123K	$P2_12_12_1$	5.823	11.246	23.559	90	90	90	3.337	
	refined with DASH	$P2_12_12_1$	5.843	11.278	23.518	90	90	90		
Epd2CB wet	refined with DASH	$P2_12_12_1$	5.856	11.296	23.560	90	90	90	1.384	
Epd2NB dry	SXD at 123K	C2	24.191	7.287	9.293	90	96.602	90	5.922	
	refined with DASH	C2	24.346	7.271	9.335	90	96.384	90		

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
Epd2NB wet	refined with DASH	C2	24.329	7.269	9.326	90	96.396	90	2.793	
Epd3CB dry	SXD at 123K	C2	23.787	5.874	11.965	90	93.311	90	2.326	
	refined with DASH	C2	23.862	5.901	12.044	90	90.743	90		
Epd3CB wet	refined with DASH	C2	23.923	5.917	12.072	90	93.746	90	2.374	
Epd4AB dry	SXD at 123K	$P2_1$	11.151	5.814	12.075	90	91.564	90	14.059	
	refined with DASH	$P2_1$	11.233	5.858	12.129	90	91.373	90		some impurity
Epd4AB wet	refined with DASH	$P2_1$	11.231	5.853	12.121	90	91.373	90	17.312	some impurity
EPd4CB dry	SXD at 123K	$P2_1$	5.722	13.442	10.474	90	99.448	90	2.862	
	refined with DASH	$P2_1$	5.732	13.449	10.575	90	99.45	90		
Epd4CB wet	refined with DASH	$P2_1$	5.740	13.468	10.579	90	99.458	90	1.289	
Epd4HBS dry	SXD at 123K	$P2_12_12_1$	9.281	9.560	19.180	90	90	90	2.385	
	refined with DASH	$P2_12_12_1$	9.358	9.579	19.334	90	90	90		
Epd4HBS wet	refined with DASH	$P2_12_12_1$	9.377	9.602	19.368	90	90	90	4.691	
EPd4NB	SXD at 123K	$P2_1$	7.968	5.960	16.908	90	91.761	90	no match	mix of Epd4NB and Epd4NB2
Epd4NB2	SXD at 123K	$P2_12_12_1$	5.517	13.301	21.991	90	90	90		
dry	refined with DASH									
Epd4NB wet	refined with DASH	$P2_12_12_1$	5.577	13.338	22.228	90	90	90	6.6837	fits Epd4NB2
EPdBr dry	SXD at 123K	$P2_1$	7.463	6.218	12.545	90	100.975	90	1.999	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	$P2_1$	7.525	6.184	12.687	90	100.721	90		
EpdBr wet	refined with DASH	$P2_1$	7.522	6.185	12.681	90	100.752	90	2.723	
EpdBS dry	SXD at 123K	$P2_1$	5.721	20.834	6.919	90	98.409	90	5.37	
	refined with DASH	$P2_1$	5.743	20.877	6.891	90	97.556	90		
EpdBS wet	refined with DASH	$P2_1$	5.758	20.931	6.909	90	97.578	90	4.261	
EpdCl dry	SXD at 123K	$P2_1$	7.256	6.123	12.549	90	102.223	90	2.068	
	refined with DASH	$P2_1$	7.269	6.098	12.558	90	102.055	90		
EpdCl wet	refined with DASH	$P2_1$	7.230	6.123	12.604	90	102.07	90	1.617	
EpdEDS dry	SXD at 123K	$P2_1$	5.711	34.065	6.659	90	90.09	90	2.777	
	refined with DASH	$P2_1$	5.718	34.084	6.652	90	90.213	90		
EpdEDS wet	refined with DASH	$P2_1$	5.711	34.030	6.641	90	90.199	90	2.086	
EpdEtSO3 dry	SXD at 123K	$P2_12_12_1$	5.488	11.906	22.639	90	90	90	3.098	
	refined with DASH	$P2_12_12_1$	5.523	12.081	22.455	90	90	90		
EpdEtSO3 wet	refined with DASH	$P2_12_12_1$	5.515	12.058	22.420	90	90	90	1.463	
EpdI dry	SXD at 123K	$P2_12_12_1$	7.317	18.893	25.599	90	90	90	1.024	
	refined with DASH	$P2_12_12_1$	7.342	19.089	25.715	90	90	90		
EpdI wet	refined with DASH	$P2_12_12_1$	7.317	18.893	25.599	90	90	90	no match	
EpdLMD dry	SXD at 123K	C2	18.027	6.493	13.776	90	92.554	90	6.597	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	C2	18.068	6.504	13.837	90	92.052	90		
EpdLMD wet	refined with DASH	C2	18.129	6.549	13.885	90	92.106	90	2.136	
EpdLTar dry	SXD at 123K	$P2_12_12_1$	6.622	7.462	33.216	90	90	90	no match	
	refined with DASH	$P2_12_12_1$	6.622	7.462	33.216	90	90	90		
EpdLTar wet	refined with DASH	$P2_12_12_1$	6.674	7.473	33.335	90	90	90	10.93	Fits EpdLTar2
EpdMale dry	SXD at 123K	$P2_12_12_1$	5.637	13.495	20.525	90	90	90	no match	
	refined with DASH	$P2_12_12_1$	5.637	13.495	20.525	90	90	90		
EpdMale wet	refined with DASH	$P2_12_12_1$	5.653	13.650	20.405	90	90	90	1.957	
EPdMalon dry	SXD at 123K	C2	15.119	5.784	13.879	90	105.765	90	2.519	
	refined with DASH	C2	15.120	5.823	13.816	90	106.207	90		
EpdMalon wet	refined with DASH	C2	15.144	5.844	13.888	90	105.517	90	1.646	
EpdMeSO3 dry	SXD at 123K	C2	14.287	6.108	14.993	90	93.211	90	1.911	
	refined with DASH	C2	14.198	6.040	14.959	90	93.214	90		
EpdMeSO3 wet	refined with DASH	C2	14.197	6.035	14.954	90	93.213	90	1.527	
EpdmTol dry	SXD at 123K	C2	23.647	5.887	12.072	90	93.053	90	4.375	
	refined with DASH	C2	23.714	5.934	12.235	90	93.647	90		
EpdmTol wet	refined with DASH	C2	23.727	5.940	12.241	90	93.64	90	3.314	
EpdRMD dry	SXD at 123K	C2	18.017	6.529	13.773	90	92.822	90	no match	

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	C2	18.017	6.529	13.773	90	92.822	90		
EpdRMD wet	refined with DASH	C2	18.113	6.528	13.853	90	92.248	90	3.602	
EpdSO4 dry	SXD at 123K	C2	30.997	6.986	5.617	90	93.354	90	4.503	
	refined with DASH	C2	33.191	6.881	5.662	90	93.155	90		
EpdSO4 wet	refined with DASH	C2	30.997	6.986	5.617	90	93.354	90	no match	

Table B.9 X-raypowder analysis for (-)pseudoephedrinium salts

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
PEpd2CB dry	SXD at 123K	$P2_1$	7.890	8.308	13.208	90	96.246	90	2.043
	refined with DASH	$P2_1$	7.913	8.345	13.304	90	95.742	90	
PEpd2CB wet	refined with DASH	$P2_1$	7.912	8.340	13.299	90	95.723	90	1.672
PEpd2HB dry	SXD at 123K	$P2_1$	7.625	8.118	13.049	90	103.124	90	6.865
	refined with DASH	$P2_1$	7.672	8.193	13.135	90	103.978	90	
PEpd2HB wet	refined with DASH	$P2_1$	7.664	8.188	13.122	90	103.984	90	6.172
PEpd2NB dry	SXD at 123K	$P2_1$	9.049	7.494	27.549	90	93.566	90	no match
	refined with DASH	$P2_1$	9.049	7.494	27.549	90	93.566	90	
PEpd2NB wet	refined with DASH	$P2_1$	9.149	7.548	27.703	90	95.533	90	1.908

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
PEpd3HB dry	SXD at 123K	C2	17.141	7.854	13.518	90	101.676	90	10.149
	refined with DASH	C2	17.391	7.788	13.505	90	100.466	90	
PEpd3HB wet	refined with DASH	C2	17.416	7.783	13.519	90	100.452	90	4.614
PEpd4CB dry	SXD at 123K	$P2_1$	7.317	8.116	14.412	90	95.960	90	no match
	refined with DASH	$P2_1$	7.317	8.116	14.412	90	95.960	90	
PEpd4CB wet	refined with DASH	$P2_1$	7.317	8.116	14.412	90	95.960	90	no match
PEpd4FB dry	SXD at 123K	$P2_1$	9.480	7.017	12.799	90	102.364	90	15.511
	refined with DASH	$P2_1$	9.578	7.071	12.865	90	102.387	90	
PEpd4FB wet	refined with DASH	$P2_1$	9.572	7.066	12.858	90	102.407	90	5.185
PEpd4HBS dry	SXD at 123K	$P2_12_12_1$	6.777	14.068	17.523	90	90	90	5.375
	refined with DASH	$P2_12_12_1$	6.754	13.983	17.808	90	90	90	
PEpd4HBS wet	refined with DASH	$P2_12_12_1$	6.766	14.007	17.819	90	90	90	1.524
PEpd4NB dry	SXD at 123K	P1	6.108	7.281	18.747	98.637	91.223	91.620	8.653
	refined with DASH	P1	6.135	7.360	18.838	97.782	90.765	91.552	
PEpd4NB wet	refined with DASH	P1	6.145	7.374	18.873	97.776	90.765	91.554	13.223
PEpdAdp dry	SXD at 123K	$P2_1$	6.824	16.198	7.759	90	93.84	90	no match
	refined with DASH	$P2_1$	6.824	16.198	7.759	90	93.84	90	
PEpdAdp wet	refined with DASH	$P2_1$	6.824	16.198	7.759	90	93.84	90	no match

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
PEpdBr dry	SXD at 123K	$P2_12_12_1$	6.753	6.918	24.013	90	90	90	4.877
	refined with DASH	$P2_12_12_1$	6.816	6.875	24.042	90	90	90	
PEpdBr wet	refined with DASH	$P2_12_12_1$	6.819	6.885	24.066	90	90	90	4.468
PEpdBS dry	SXD at 123K	$P2_12_12_1$	6.776	8.058	30.198	90	90	90	6.352
	refined with DASH	$P2_12_12_1$	6.823	8.103	30.151	90	90	90	
PEpdBS wet	refined with DASH	$P2_12_12_1$	6.863	8.150	30.321	90	90	90	4.103
PEpdCl dry	SXD at 123K	$P2_12_12_1$	25.358	6.428	6.901	90	90	90	
	refined with DASH	$P2_12_12_1$	25.275	6.395	6.838	90	90	90	3.49
PEpdCl wet	refined with DASH	$P2_12_12_1$	25.334	6.411	6.859	90	90	90	1.627
PEpdEDS dry	SXD at 123K	$P2_1$	5.528	18.831	16.947	90	91.228	90	2.012
	refined with DASH	$P2_1$	5.575	18.960	16.989	90	91.407	90	
PEpdEDS wet	refined with DASH	$P2_1$	5.556	18.939	16.969	90	91.468	90	1.183
PEpdLTar dry	SXD at 123K	$P2_12_12_1$	7.558	7.606	28.374	90	90	90	6.114
	refined with DASH	$P2_12_12_1$	7.564	7.567	28.534	90	90	90	
PEpdLTar wet	refined with DASH	$P2_12_12_1$	7.568	7.543	28.503	90	90	90	2.464
PEpdMale dry	SXD at 123K	$P2_1$	5.593	12.922	9.761	90	93.918	90	2.907
	refined with DASH	$P2_1$	5.590	12.993	9.855	90	93.331	90	
PEpdMale wet	refined with DASH	$P2_1$	5.579	12.973	9.834	90	93.343	90	1.764

Structure	Source of unit cell	Sp G	Cell parameters						Goodness of fit (Chi^2)
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	
PEpdoTol dry	SXD at 123K	$P2_1$	7.974	8.260	13.237	90	95.780	90	3.209
	refined with DASH	$P2_1$	8.003	8.318	13.432	90	95.022	90	
PEpdoTol wet	refined with DASH	$P2_1$	8.003	8.319	13.431	90	95.050	90	6.024
PEpdRMal dry	SXD at 123K	$P2_12_12_1$	7.369	8.252	24.896	90	90	90	6.095
	refined with DASH	$P2_12_12_1$	7.341	8.280	24.888	90	90	90	
PEpdRMal wet	refined with DASH	$P2_12_12_1$	7.304	8.328	25.075	90	90	90	1.12
PEpdLTar dry	SXD at 123K	$P2_12_12_1$	7.558	7.606	28.374	90	90	90	no match
	refined with DASH	$P2_12_12_1$	7.558	7.606	28.374	90	90	90	
PEpdRTar wet	refined with DASH	$P2_12_12_1$	7.558	7.606	28.374	90	90	90	no match
PEpdSO4 dry	SXD at 123K	$P2_12_12_1$	6.803	12.003	16.334	90	90	90	7.415
	refined with DASH	$P2_12_12_1$	6.828	11.990	16.286	90	90	90	
PEpdSO4 wet	refined with DASH	$P2_12_12_1$	6.850	12.070	16.367	90	90	90	2.083

Table Error! No text of specified style in document.**.10** X-ray powder analysis for (-)methylephedrinium salts

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MEpd2AB dry	SXD at 123K	$P2_1$	6.924	13.856	8.769	90	97.216	90	5.576	

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	$P2_1$	6.842	14.258	8.886	90	95.937	90		
MEpd2AB wet	refined with DASH	$P2_1$	6.845	14.256	8.892	90	96.089	90	3.798	
MEpd2CB dry	SXD at 123K	$P2_1$	6.148	13.135	10.598	90	99.160	90	no match	
	refined with DASH	$P2_1$	6.148	13.135	10.598	90	99.160	90		
MEpd2CB wet	refined with DASH	$P2_1$	6.148	13.135	10.598	90	99.160	90	no match	
MEpd2FB dry	SXD at 123K	$P2_1$	5.729	14.824	9.721	90	97.952	90	3.774	
	refined with DASH	$P2_1$	5.827	14.774	9.801	90	97.583	90		
MEpd2FB wet	refined with DASH	$P2_1$	5.806	14.728	9.766	90	97.579	90	2.199	
MEpd2HB dry	SXD at 123K	$P2_12_12_1$	9.443	11.644	15.068	90	90	90	2.871	
	refined with DASH	$P2_12_12_1$	9.549	11.692	15.223	90	90	90		
MEpd2HB wet	refined with DASH	$P2_12_12_1$	9.539	11.682	15.217	90	90	90	5.125	
MEpd2NB dry	SXD at 123K	$P2_1$	5.812	13.178	12.041	90	103.222	90	3.787	
	refined with DASH	$P2_1$	5.857	13.239	12.045	90	103.499	90		
MEpd2NB wet	refined with DASH	$P2_1$	5.875	13.266	12.046	90	103.484	90	3.074	
MEpd3AB dry	SXD	$P2_1$	5.823	13.443	21.092	90	95.723	90	16.130	
	refined with DASH	$P2_1$	5.885	13.516	21.096	90	95.754	90		
MEpd3AB wet	refined with DASH	$P2_1$	5.878	13.509	21.087	90	95.621	90	5.998	

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MEpd3CB dry	SXD at 123K	$P2_12_12_1$	6.647	11.997	23.039	90	90	90		
	refined with DASH	$P2_12_12_1$	6.632	12.047	23.266	90	90	90	3.004	
MEpd3CB wet	refined with DASH	$P2_12_12_1$	6.606	12.024	23.233	90	90	90	8.429	
MEPD3FB dry	SXD at 123K	$P2_1$	5.832	13.011	10.898	90	97.971	90	5.214	
	refined with DASH	$P2_1$	5.922	13.122	10.888	90	98.277	90		
MEpd3FB wet	refined with DASH	$P2_1$	5.916	13.116	10.884	90	98.259	90	6.689	
MEpd4AB dry	SXD at 123K	$P2_12_12_1$	9.279	13.303	13.880	90	90	90	5.797	
	refined with DASH	$P2_12_12_1$	9.445	12.312	13.758	90	90	90		
MEpd4AB wet	refined with DASH	$P2_12_12_1$	9.456	13.345	13.787	90	90	90	4.968	
MEpd4CB dry	SXD at 123K	$P2_1$	5.992	14.204	9.900	90	96.679	90	2.233	
	refined with DASH	$P2_1$	6.032	14.315	9.953	90	96.846	90		
MEpd4CB wet	refined with DASH	$P2_1$	6.030	14.310	98.949	90	96.837	90	2.445	
MEpd4HB dry	SXD at 123K	$P2_1$	12.825	7.724	18.065	90	104.569	90	3.224	
	refined with DASH	$P2_1$	12.873	7.708	18.120	90	104.272	90		
MEpd4HB wet	refined with DASH	$P2_1$	12.888	7.717	18.149	90	104.375	90	2.137	
MEpd4HBS dry	SXD at 123K	$P2_1$	6.140	13.373	10.300	90	98.217	90	6.94	
	refined with DASH	$P2_1$	6.195	13.357	10.366	90	98.113	90		

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MEpd4HBS wet	refined with DASH	$P2_1$	6.204	13.397	10.388	90	98.099	90	6.494	
MEpd4NB dry	SXD at 123K	$P2_1$	5.831	12.970	23.552	90	94.839	90	4.549	
	refined with DASH	$P2_1$	5.876	12.974	23.482	90	94.325	90		
MEpd4NB wet	refined with DASH	$P2_1$	5.873	12.986	23.516	90	94.450	90	1.247	
MEpdBF4 dry	SXD at 123K	$P2_12_12_1$	7.884	11.445	14.518	90	90	90	6.418	
	refined with DASH	$P2_12_12_1$	7.902	11.571	14.534	90	90	90		
MEpdBF4 wet	refined with DASH	$P2_12_12_1$	7.947	11.618	14.578	90	90	90	8.78	
MEpdBr dry	SXD at 123K	$P2_12_12_1$	7.285	9.667	17.254	90	90	90	3.984	
	refined with DASH	$P2_12_12_1$	7.353	9.738	17.222	90	90	90		
MEpdBr wet	refined with DASH	$P2_12_12_1$	7.358	9.743	17.248	90	90	90	3.999	
MEpdBS dry	SXD at 123K	$P2_1$	7.423	11.236	10.568	90	93.590	90	4.782	
	refined with DASH	$P2_1$	7.428	11.329	10.594	90	93.899	90		
MEpdBS wet	refined with DASH	$P2_1$	7.423	11.236	10.568	90	93.590	90	no match	
MEpdBz dry	SXD at 123K	$P2_12_12_1$	8.628	10.992	18.791	90	90	90		
	refined with DASH	$P2_12_12_1$	8.622	11.081	18.945	90	90	90	8.887	
MEpdBz wet	refined with DASH	$P2_12_12_1$	8.616	11.048	18.902	90	90	90	10.174	
MEpdCl dry	SXD at 123K	$P2_12_12_1$	7.156	9.571	16.863	90	90	90	3.955	

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	refined with DASH	$P2_12_12_1$	7.208	9.626	16.867	90	90	90		
MEpdCl wet	refined with DASH	$P2_12_12_1$	7.293	9.306	17.048	90	90	90	8.271	
MEpdEDS dry	SXD at 123K	$P2_1$	5.922	32.974	7.159	90	99.465	90	6.188	
	refined with DASH	$P2_1$	5.964	32.648	7.220	90	99.660	90		
MEpdEDS wet	refined with DASH	$P2_1$	5.985	33.057	7.241	90	99.242	90	1.608	
MEpdEtSO3 dry	SXD at 123K	C2	15.324	5.971	16.206	90	94.995	90	4.485	
	refined with DASH	C2	15.334	6.007	16.427	90	94.962	90		
MEpdEtSO3 wet	refined with DASH	C2	15.324	5.971	16.206	90	94.995	90	no match	
MEpdI dry	SXD at 123K	$P2_1$	7.642	25.507	7.878	90	104.173	90	3.491	
	refined with DASH	$P2_1$	7.649	26.198	7.893	90	104.936	90		
MEpdI wet	refined with DASH	$P2_1$	7.652	25.864	7.787	90	105.355	90	2.135	
MEpdLMD dry	SXD at 123K	$P2_12_12_1$	7.410	9.821	23.984	90	90	90	5.415	
	refined with DASH	$P2_12_12_1$	7.433	9.861	24.206	90	90	90		
MEpdLMD wet	refined with DASH	$P2_1$	10.036	5.790	16.023	90	93.246	90	4.211	fits RMEpdLMD2
MEpdLTar dry	SXD at 123K	$P2_1$	10.698	7.466	11.636	90	112.490	90	4.924	
	refined with DASH	$P2_1$	10.772	7.459	11.717	90	112.938	90		
MEpdLTar wet	refined with DASH	$P2_1$	10.747	7.444	11.692	90	112.954	90	2.374	

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MEpdMale dry	SXD at 123K	$P2_12_12_1$	19.966	13.508	5.776	90	90	90	2.948	
	refined with DASH	$P2_12_12_1$	19.976	13.652	5.830	90	90	90		
MEpdMale wet	refined with DASH	$P2_12_12_1$	19.972	13.639	5.830	90	90	90	5.126	
MEpdMalon dry	SXD at 123K	P1	7.839	9.697	11.201	103.350	100.240	111.083	2.829	
	refined with DASH	P1	7.903	9.712	11.375	103.479	100.560	111.582		
MEpdMalon wet	refined with DASH	P1	7.930	9.727	11.447	103.152	100.514	111.785	9.076	
MEpdMeSO3 dry	SXD at 123K	$P2_12_12_1$	5.880	21.637	33.840	90	90	90	no match	
	refined with DASH	$P2_12_12_1$	5.880	21.637	33.840	90	90	90		
MEpdMeSO3 wet	refined with DASH	$P2_12_12_1$	5.880	21.637	33.840	90	90	90	no match	
MEpdoTol dry	SXD at 123K	$P2_1$	5.940	15.020	9.691	90	97.506	90	5.495	
	refined with DASH	$P2_1$	6.032	14.971	9.705	90	97.314	90		
MEpdoTol wet	refined with DASH	$P2_1$	6.056	15.009	9.715	90	97.322	90	2.22	
MEpdpTol dry	SXD at 123K	$P2_1$	6.044	14.126	9.936	90	98.017	90	5.272	
	refined with DASH	$P2_1$	6.111	14.246	10.027	90	97.959	90		
MEPDpTol wet	refined with DASH	$P2_1$	6.091	14.206	9.993	90	97.964	90	4.608	
MEpdRMD dry	SXD at 123K	$P2_12_12_1$	7.426	9.835	23.950	90	90	90	no match	conglomerate
	refined with DASH	$P2_12_12_1$	7.426	9.835	23.950	90	90	90		

Structure	Source of unit cell	Unit cell parameters							Goodness of fit (Chi^2)	Comment
		Sp Gr	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
MEpdRMD wet	refined with DASH	$P2_12_12_1$	7.459	9.923	24.201	90	90	90	4.989	fits MEpdLMD
MEpdSuc dry	SXD at 123K	$P2_12_12_1$	6.094	14.060	17.880	90	90	90	3.317	
	refined with DASH	$P2_12_12_1$	6.154	14.164	17.879	90	90	90		
MEpdSuc wet	refined with DASH	$P2_12_12_1$	6.144	14.152	17.864	90	90	90	1.673	

Table B.1 X-ray powder analysis for (+/-)methylephedrinium salts

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
RMEpd dry	SXD at 123K	$P2_12_12_1$	8.075	8.899	14.571	90	90	90	4.528	conglomerate
	Refined with DASH	$P2_12_12_1$	14.703	8.922	8.090	90	90	90		chiral as expected
RMEpd wet	Refined with DASH	$P2_12_12_1$	14.497	8.920	8.092	90	90	90	4.926	chiral as expected
RMEpd2AB dry	SXD at 123K	$Pbc2_1$	41.939	7.997	10.243	90	90	90	2.965	
	Refined with DASH	$Pbc2_1$	42.218	8.033	10.221	90	90	90		
RMEpd2AB wet	Refined with DASH	$Pbc2_1$	41.939	7.997	10.243	90	90	90	no match	
RMEpd2CB dry	SXD at 123K	$Pca2_1$	10.418	8.037	20.250	90	90	90	2.566	
	Refined with DASH	$Pca2_1$	10.561	8.075	20.336	90	90	90		
RMEpd2CB wet	Refined with DASH	$Pca2_1$	10.531	8.054	20.288	90	90	90	2.315	

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
RMEpd2FB dry	SXD at 123K	$P2_1$	5.729	14.824	9.721	90	97.952	90	3.075	conglomerate
	Refined with DASH	$P2_1$	5.835	14.797	9.816	90	97.597	90		chiral as expected
RMEpd2FB wet	Refined with DASH	$P2_1$	5.729	14.824	9.721	90	97.952	90	no match	
RMEpd2NB dry	SXD at 123K	Pbca	15.646	11.214	21.061	90	90	90	2.78	
	Refined with DASH	Pbca	15.659	11.210	21.231	90	90	90		
RMEpd2NB wet	Refined with DASH	Pbca	15.646	11.214	21.061	90	90	90	no match	
RMEpd3CBdry	SXD at 123K	C2/c	24.787	5.849	23.708	90	97.920	90	3.306	
	Refined with DASH	C2/c	24.734	5.968	23.821	90	97.723	90		
RMEpd3CB wet	Refined with DASH	C2/c	24.711	5.963	23.803	90	97.701	90	3.62	
RMEpd3FB dry	SXD at 123K	C2/c	24.219	5.748	23.750	90	96.799	90	2.95	
	Refined with DASH	C2/c	24.259	5.858	23.875	90	96.897	90		
RMEpd3FB wet	Refined with DASH	C2/c	24.189	5.837	23.795	90	96.884	90	6.093	
RMEpd3HB dry	SXD at 123K	$P2_1/c$	10.254	14.978	11.250	90	92.194	90	4.852	
	Refined with DASH	$P2_1/c$	10.353	14.843	11.406	90	92.684	90		
RMEpd3HB wet	Refined with DASH	$P2_1/c$	10.342	14.831	11.403	90	92.610	90	1.622	
RMEpd3NB dry	SXD at 123K	C2/c	25.322	5.767	23.695	90	96.453	90	4.432	
	Refined with DASH	C2/c	25.199	5.869	23.743	90	96.758	90		
RMEpd3NB wet	Refined with DASH	C2/c	25.249	5.882	23.784	90	96.75	90	2.851	

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
RMEpd4AB dry	SXD at 123K	Pbca	9.046	14.947	24.822	90	90	90	no match	
	Refined with DASH	Pbca	9.046	14.947	24.822	90	90	90		
RMEpd4AB wet	Refined with DASH	Pbca	9.193	14.923	25.032	90	90	90	3.708	
RMEpd4CB dry	SXD at 123K	$P2_1$	5.992	14.204	9.900	90	96.679	90	3.764	conglomerate
	Refined with DASH	$P2_1$	6.038	14.324	9.966	90	96.855	90		chiral as expected
RMEpd4CB wet	Refined with DASH	$P2_1$	6.037	14.316	9.961	90	96.839	90	1.809	chiral as expected
RMEpd4FB dry	SXD at 123K	P21/c	12.537	13.444	10.367	90	105.903	90	2.379	
	Refined with DASH	$P2_1/c$	12.583	13.478	10.479	90	105.935	90		
RMEpd4FB wet	Refined with DASH	$P2_1/c$	12.577	13.485	10.476	90	105.928	90	2.399	
RMEpd4HB dry	SXD at 123K	$P2_1$	12.825	7.724	18.065	90	104.569	90	5.425	conglomerate
	Refined with DASH	$P2_1$	12.895	7.702	18.163	90	104.403	90		chiral as expected
RMEpd4HB wet	Refined with DASH	$P2_1$	12.876	7.712	18.148	90	104.374	90	1.252	chiral as expected
RMEpd4HBS wet	SXD at 123K	P-1	10.218	13.641	15.004	64.086	87.575	72.856	2.67	
	Refined with DASH	P-1	10.249	13.723	15.105	63.728	87.635	72.55		
RMEpd4HBS wet	Refined with DASH	P-1	10.248	13.709	15.090	63.844	89.769	72.735	5.883	
RMEpd4NB dry	SXD at 123K	$P2_1/c$	5.828	12.811	23.307	90	91.683	90	2.99	
	Refined with DASH	$P2_1/c$	5.830	12.841	23.565	90	90.952	90		
RMEpd4NB wet	Refined with DASH	$P2_1/c$	5.873	12.888	23.214	90	90.685	90	7.442	

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
RMEpdAdp dry	SXD at 123K	$P2_1/c$	5.854	23.783	12.620	90	103.349	90	3.926	
	Refined with DASH	$P2_1/c$	5.890	23.980	12.680	90	102.126	90		
RMEpdAdp wet	Refined with DASH	$P2_1/c$	5.892	24.006	12.719	90	102.073	90	1.435	
RMEpdBr dry	SXD at 123K	$P2_1/c$	5.738	30.598	6.982	90	106.92	90	6.312	
	Refined with DASH	$P2_1/c$	5.801	31.000	7.016	90	107.183	90		
RMEpdBr wet	Refined with DASH	$P2_1/c$	5.801	30.985	7.010	90	107.173	90	3.137	
RMEpdBS RMEPdBS2 dry	SXD at 123K	P-1	5.831	9.271	17.179	79.604	85.506	80.861	no match	
	SXD at 123K	$P2_1/c$	10.428	10.843	14.967	90	94.601	90		
	Refined with DASH	P-1	5.831	9.271	17.179	79.604	85.506	80.861		
RMEpdBS wet	Refined with DASH	$P2_1/c$	10.341	10.907	14.796	90	94.602	90	1.822	fits RMEpdBS2
RMEpdBz dry	SXD at 123K	Pbca	13.928	11.220	20.700	90	90	90	4.093	
	Refined with DASH	Pcbca	13.983	11.323	20.858	90	90	90		
RMEpdBz wet	Refined with DASH	$P2_12_12_1$	8.620	11.062	18.928	90	90	90	1.869	fits MEpdBz
RMEpdCl dry	SXD at 123K	C2/c	33.603	6.986	9.909	90	95.085	90	3.081	
	Refined with DASH	C2/c	33.545	7.024	9.970	90	95.361	90		
RMEpdCl wet	Refined with DASH	C2/c	33.687	7.056	10.017	90	95.376	90	3.350	
RMEpdEDS	SXD at 123K	$P2_1/c$	5.939	33.056	7.307	90	102.924	90	1.579	
RMEpdEDS2	SXD at 123K	P-1	5.771	10.606	13.046	106.273	99.721	103.95		

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
dry	Refined with DASH	$P2_1/c$	5.967	33.072	7.399	90	103	90		
RMEpdEDS wet	Refined with DASH	P-1	5.784	10.681	13.009	106.186	99.645	104.241	1.451	fits RMEPDEDS2
RMEpdI dry	SXD at 123K	C2/c	12.731	8.988	24.957	90	96.364	90	2.424	
	Refined with DASH	C2/c	12.773	9.169	25.075	90	96.648	90		fits RMEpdI2
RMEpdI wet	Refined with DASH	C2/c	13.059	9.299	25.657	90	95.547	90	6.652	fits RMEpdI2
RMEpdLMD dry	SXD at 123K	$P2_12_12_1$	7.373	9.774	23.967	90	90	90	no match	
	Refined with DASH	$P2_12_12_1$	7.373	9.774	23.967	90	90	90		
RMEpdLMD wet	Refined with DASH	$P2_12_12_1$	7.373	9.774	23.967	90	90	90	no match	
RMEpdMale dry	SXD at 123K	$P2_1/c$	10.667	24.555	5.921	90	100.111	90	3.554	
	Refined with DASH	$P2_1/c$	10.561	24.918	5.952	90	99.823	90		
RMEpdMale wet	Refined with DASH	$P2_1/c$	10.594	25.002	5.971	90	99.792	90	1.461	
RMEpdMalon dry	SXD at 123K	P-1	10.194	5.708	13.204	71.637	80.822	81.117	no match	
	Refined with DASH	P-1	10.194	5.708	13.204	71.637	80.822	81.117		
RMEpdMalon wet	Refined with DASH	P-1	10.166	5.845	13.193	71.028	81.799	79.872	12.789	
RMEpdMeSO32 dry	SXD at 123K	$P2_1$	5.762	17.481	13.701	90	95.417	90		
	Refined with DASH	$P2_1$	5.821	17.735	13.749	90	96.307	90	3.715	fits RMEpdMeSO32
RMEpdMeSO3 wet	Refined with DASH	$P2_1$	5.822	17.736	13.738	90	96.261	90	2.558	fits RMEpdMeSO32
RMEpdmTol dry	SXD at 123K	C2/c	24.371	6.022	23.684	90	95.240	90	3.214	

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	Refined with DASH	C2/c	24.292	6.114	23.937	90	95.961	90		
RMEpdmTol wet	Refined with DASH	C2/c	24.318	6.112	23.919	90	95.977	90	6.79	
RMEpdoTol dry	SXD at 123K	$Pca2_1$	10.472	8.045	20.294	90	90	90	8.576	
	Refined with DASH	$Pca2_1$	10.598	8.067	20.419	90	90	90		
RMEpdoTol wet	Refined with DASH	$Pca2_1$	10.582	8.058	20.396	90	90	90	4.694	
RMEpdpTol dry	SXD at 123K	$P2_1$	6.044	14.126	9.936	90	98.017	90	9.838	conglomerate
	Refined with DASH	$P2_1$	6.098	14.220	10.006	90	98.006	90		chiral as expected
RMEpdpTol wey	Refined with DASH	$P2_1$	6.092	14.215	9.998	90	97.957	90	2.445	chiral as expected
RMEpdRMDdry	SXD at 123K	$P2_1/c$	13.065	9.547	13.901	90	91.572	90	7.566	
	Refined with DASH	$P2_1/c$	13.093	9.553	13.882	90	91.720	90		
RMEpdRMD wet	Refined with DASH	$P2_1/c$	13.141	9.617	13.960	90	91.780	90	3.702	
RMEpdRTar dry	SXD at 123K	$Pbc2_1$	7.913	10.144	40.028	90	90	90	6.862	
	Refined with DASH	$Pbc2_1$	7.978	10.216	39.324	90	90	90		
RMEpdRTar wet	Refined with DASH	$Pbc2_1$	7.999	10.245	40.027	90	90	90	3.091	
RMEpdSO4 dry	SXD at 123K	$P2_1/c$	5.893	17.340	14.440	90	108.546	90	4.062	
	Refined with DASH	$P2_12_12_1$	6.102	13.275	18.113	90	90	90		fits MEpdSO4
RMEpdSO4 wet	Refined with DASH	$P2_1/c$	5.893	17.340	14.440	90	108.546	90	no match	
RMEpdSuc dry	SXD at 123K	$P2_1/c$	16.065	8.128	9.764	90	92.226	90		

Structure	Source of unit cell	Sp Gr	Cell parameters						Goodness of fit (Chi^2)	Comment
			a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)		
	Refined with DASH	$P2_1/c$	16.200	8.167	9.836	90	90.956	90	25.033	impurities present
RMEpdSuc wet	Refined with DASH	$P2_1/c$	16.235	8.190	9.852	90	90.940	90	3.711	

Appendix C Testing the predictive power of the training sets

C.1 Predicting solubility for tyrammonium salts

The tyrammonium salts consists of twenty different salts that vary greatly in solubility. Figure C.1 shows the results of trying to predict the solubility with the regression training set. It can be seen that this model cannot be used to predict solubility of salts from this cation group. The classification model had some success with this group in that it was able to correctly predict all the sparingly soluble salts. Unfortunately it had little success in the prediction of the other two categories, see Table C.1

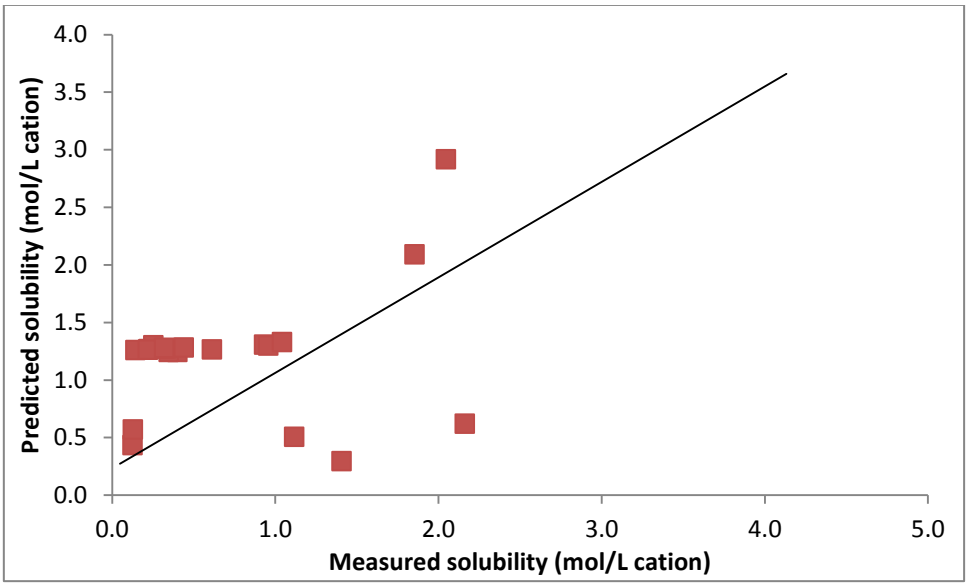

Figure C.1 Plot of measured versus predicted solubility for the prediction test set of tyrammonium salts. Line obtained from training set, **red** represents tyrammonium salts

Table C.1 Observed and predicted solubility results for the prediction test set of tyrammonium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	12	0	0	0.0
Soluble	4	1	0	80.0
Very soluble	0	1	2	33.3

C.2 Predicting solubility for phenylpropylammonium salts

This group contains only two salts of which neither lie on the prediction line of the regression training set, see Figure C. 2. Using the classification model one salts' solubility category was correctly predicted, see Table C.2.

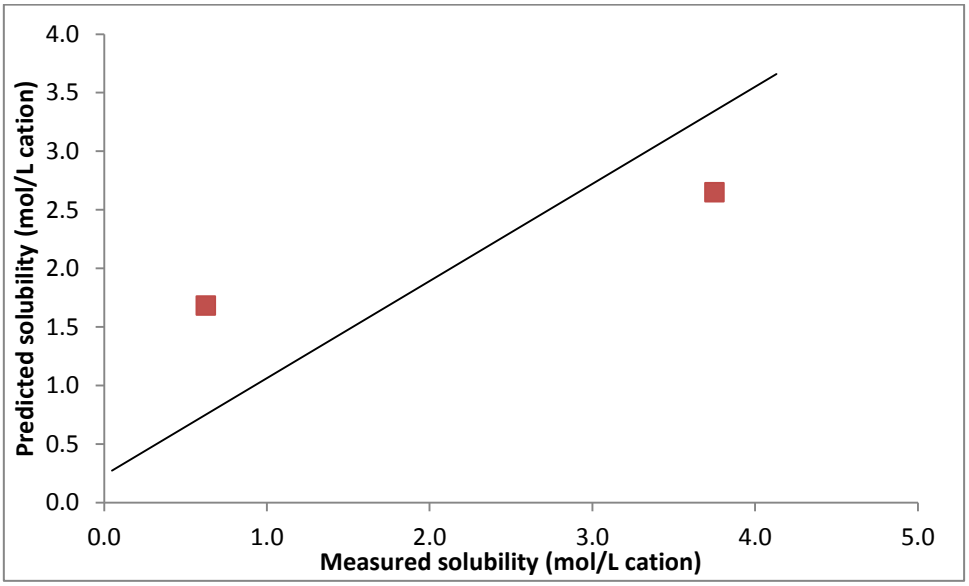

Figure C.2 Plot of measured versus predicted solubility for the prediction test set of phenylpropylammonium salts. Line obtained from training set, **red** represents phenylpropylammonium salts

Table C.2 Observed and predicted solubility results for the prediction test set of phenylpropylammonium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	0	0	1	100.0
Very soluble	0	0	1	0.0

C.3 Predicting solubility for methylphenethylaminium salts

This dataset contains ten salts of which after analysis using the classification model half of the salts were predicted into the correct solubility category, see Table C.3. The regression training set again had no consistency in prediction, see Figure C.3.

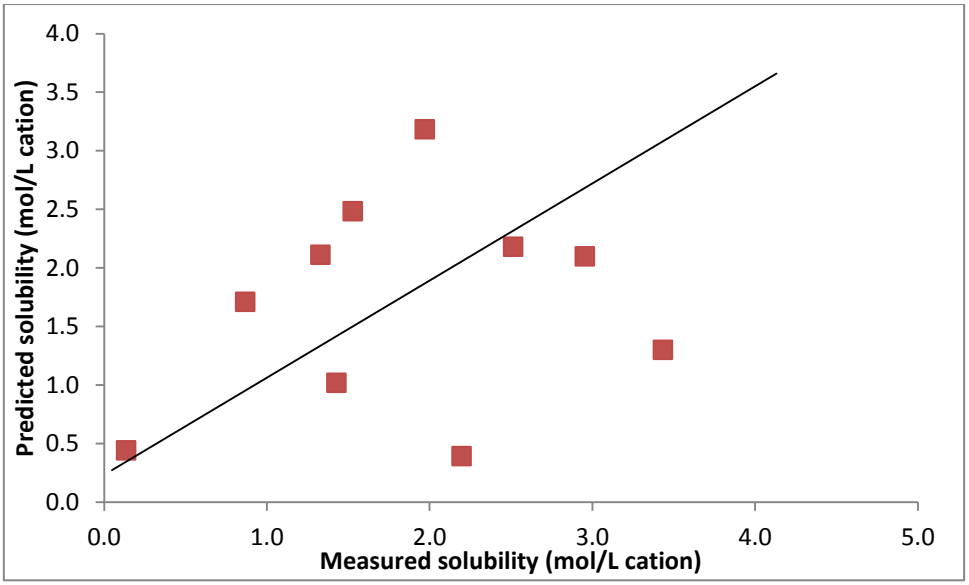

Figure C.3 Plot of measured versus predicted solubility for the prediction test set of methylphenethylaminium salts. Line obtained from training set, **red** represents methylphenethylaminium salts

Table C.3 Observed and predicted solubility results for the prediction test set of methylphenethylaminium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	1	0	0	0.0
Soluble	1	1	2	75.5
Very soluble	0	1	4	20.0

C.4 Predicting solubility for α(methylaminomethyl)benzyl alcohol salts

This group contains eight salts of which half were correctly predicted into the right solubility category with the classification prediction method, see Table C.4**Error! Reference source not found.**. The regression model appears to correctly predict the solubility of five salts, see Figure C.4. These five salts encompass all four of the benzoate derived salts and the succinate salt.

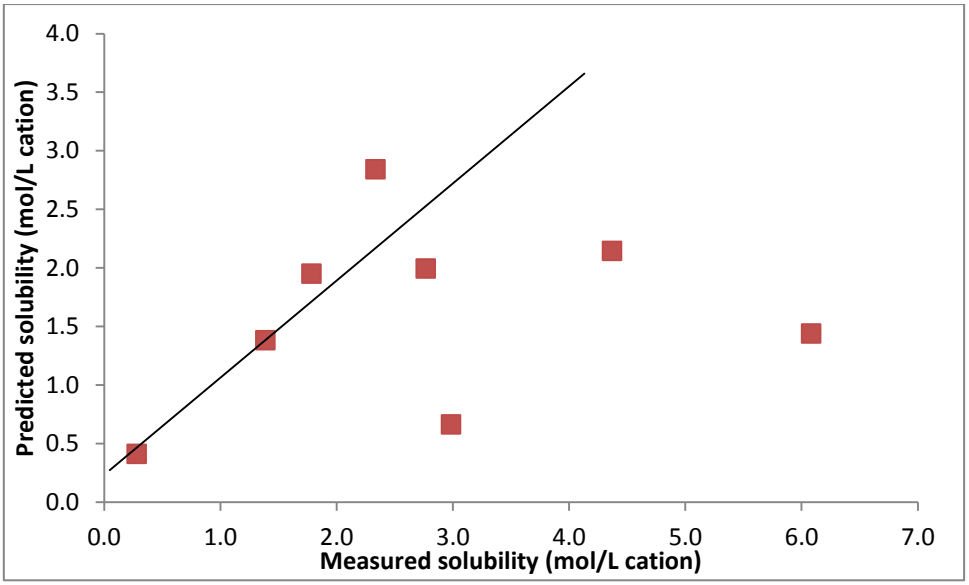

Figure C.4 Plot of measured versus predicted solubility for the prediction test set of α(methylaminomethyl)benzyl alcohol salts. Line obtained from training set, **red** represents α(methylaminomethyl)benzyl alcohol salts

Table C.4 Observed and predicted solubility results for the prediction test set of α(methylaminomethyl)benzyl alcohol salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	1	0	0	0.0
Soluble	0	1	0	0.00
Very soluble	2	2	2	66.6

C.5 Predictiing solubility for (-)ephedrinium salts

This dataset contains fourteen salts from varying solubility categories. Although the regression model is quite erratic it appears to again predict the benzoate derived salts' solubility to within a reasonable error, see Figure C.5. Table C.5 shows there observed category versus their predicted category for the salts predicted using the classification training set. The prediction of the sparingly soluble compounds has an error of 11.1 % with the incorrect prediction for one compound. Again, the other two categories show very little prediction ability.

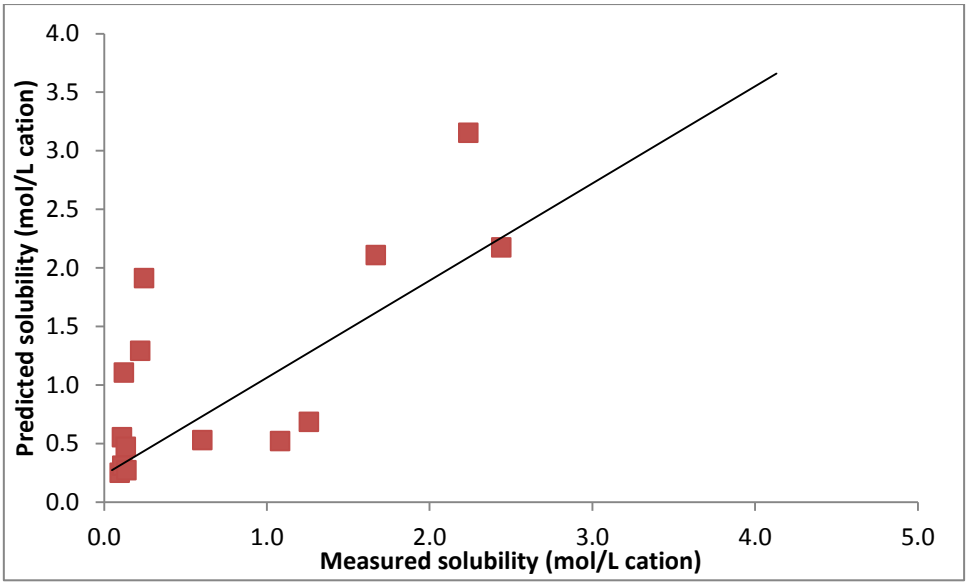

Figure C.5 Plot of measured versus predicted solubility for the prediction test set of ephedrinium salts. Line obtained from training set, **red** represents ephedrinium salts

Table C.5 Observed and predicted solubility results for the prediction test set of ephedrinium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	8	1	0	11.1
Soluble	2	1	0	66.6
Very soluble	1	0	1	50.0

C.6 Predicting solubility for (-)pseudoephedrinium salts

There are eight salts containing the (-)pseudoephedrine cation that were analysed. Similar to the above the regression analysis is able to reasonable predict the solubility of the benzoate derived salts, see Figure C.6. On the contrary the classification model has no success at correctly predicting salt solubility, see Table C.6.

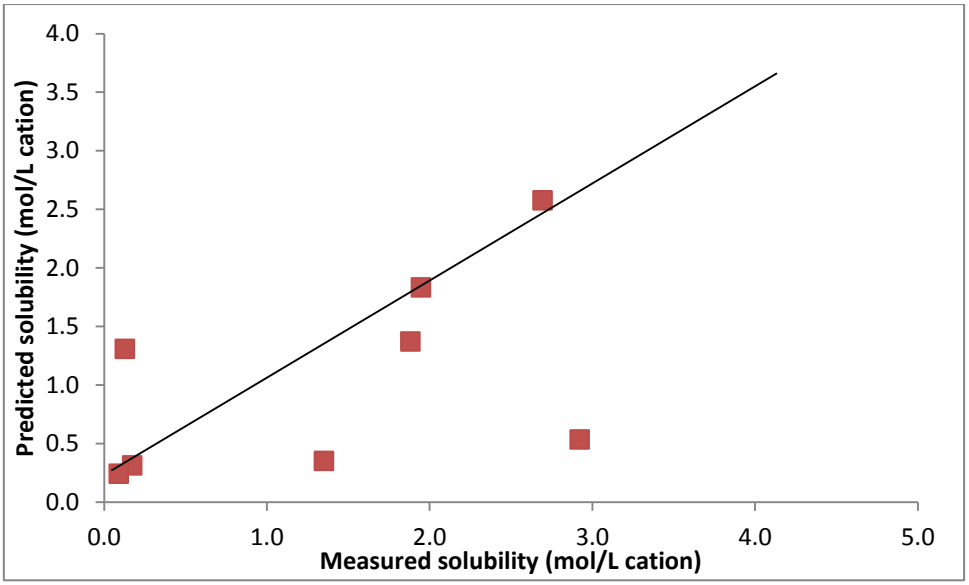

Figure C.6 Plot of measured versus predicted solubility for the prediction test set of pseudoephedrinium salts. Line obtained from training set, **red** represents psuedoephedrinium salts

Table C.6 Observed and predicted solubility results for the prediction test set of pseudoephedrinium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	1	2	0	66.6
Soluble	1	0	0	100.0
Very soluble	1	2	1	75.5

C.7 Predicting solubility for dimethylphenethylaminium salts

The final dataset to be examined was that of the five dimethylphenethylaminium salts are shown below in Figure C.7 and Table C.7. The regression model and the classification model were able to succfully predict the solubility without too much associated error.

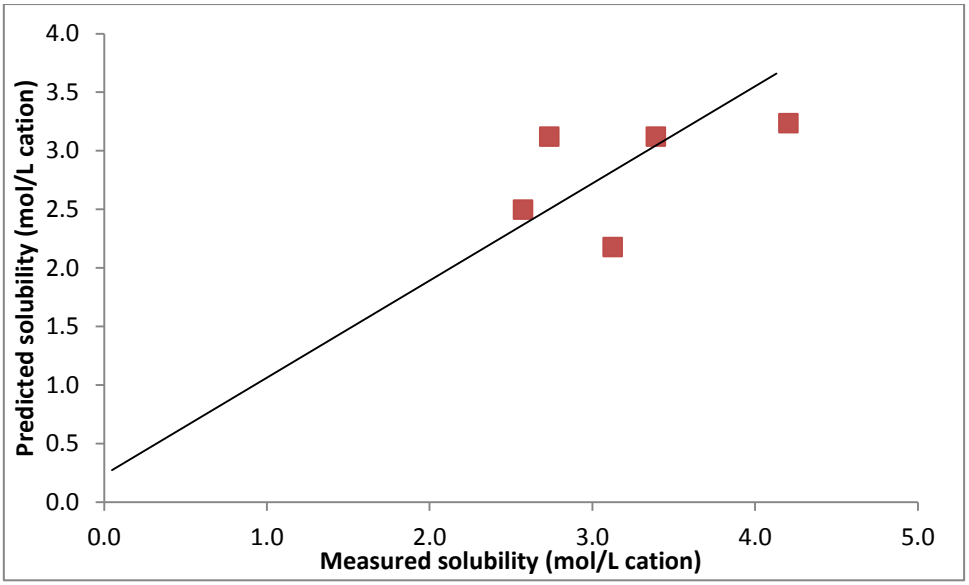

Figure C.7 Plot of measured versus predicted solubility for the prediction test set of dimethylphenethylaminium salts. Line obtained from training set, **red** represents dimethylphenethylaminium salts

Table C.7 Observed and predicted solubility results for the prediction test set of dimethylphenethylaminium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Very soluble	0	0	5	0.0

Appendix D Building of training and predicting datasets using uncorrected 2D and 3D parameters

In order to ensure that the correction of the 2D and 3D parameters did not have a negative effect on the regression and classification models or the predictability of the datasets, analysis was also performed using the uncorrected parameter values. For this the inputted 2D and 3D parameters were those of the associated free acid alone. See Section 7, Random forest.

D.1 Regression training model built with uncorrected 2D, 3D, physical and crystal parameters (RegTsetUncor.txt)

The uncorrected 2D and 3D parameters were substituted into the finalised regression training model. As the same base correction was used here for all salts the output is the same as observed for the original corrected model, see Figure D.1.

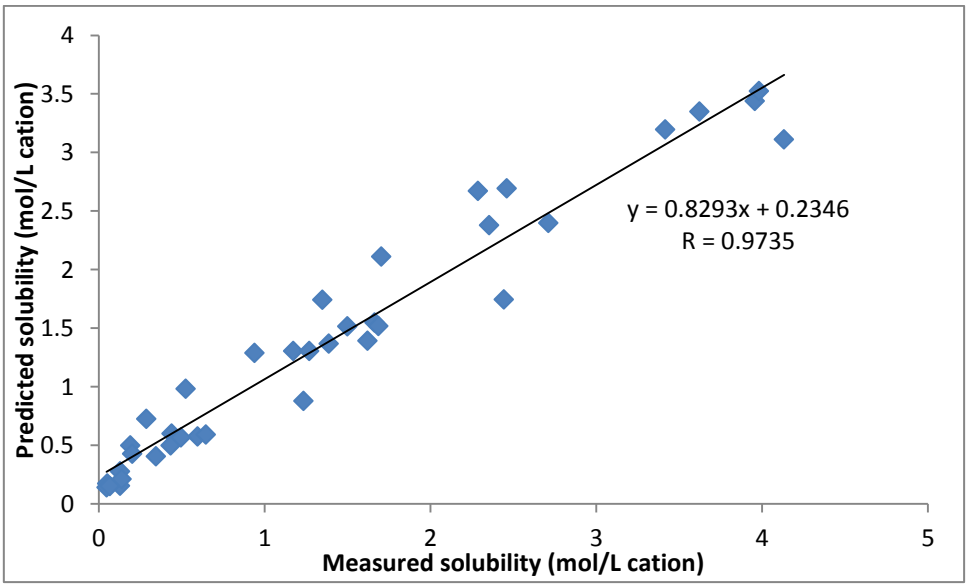

Figure D.1 Plot of measured versus predicted solubility for uncorrected regression training model

D.2 Classification training model built with uncorrected 2D, 3D, physical, and crystal parameters (ClassTsetUncor.txt)

As with the regression training model the substitution of the uncorrected 2D and 3D parameters had no effect on the classification training model, see Figure D.2 and Table D.1.

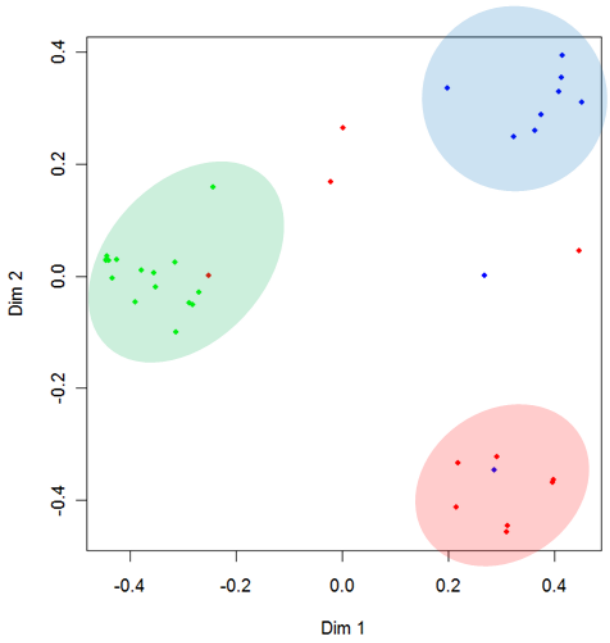

Figure D.2 Proximity matrix for uncorrected classification model. **Green** represents sparingly soluble compounds, **red** represents soluble compounds and **blue** represents very soluble compounds

Table D.1 Observed and predicted solubility results for the uncorrected classification training model

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	class error (%)
Sparingly soluble	16	0	0	0.00
Soluble	3	6	2	45.5
Very soluble	0	2	8	20.0

D.3 Testing the predictive power of the uncorrected training sets

Both the uncorrected regression and classification training sets were used to test their ability at predicting solubility for salts already tested using the corrected models. This was performed to see if the free acid 2D and 3D parameters were better at predicting solubility instead of the parameters composed from both the free acid and free base.

D.3.1 Predicting solubility for (+/-)methylephedrinium conglomerate salts using uncorrected regression and classification training sets

As expected the methylephedrinium conglomerate salts' solubility were still correctly predicted when using the uncorrected regression and classification training sets, see Figure D.3 and Table D.2.

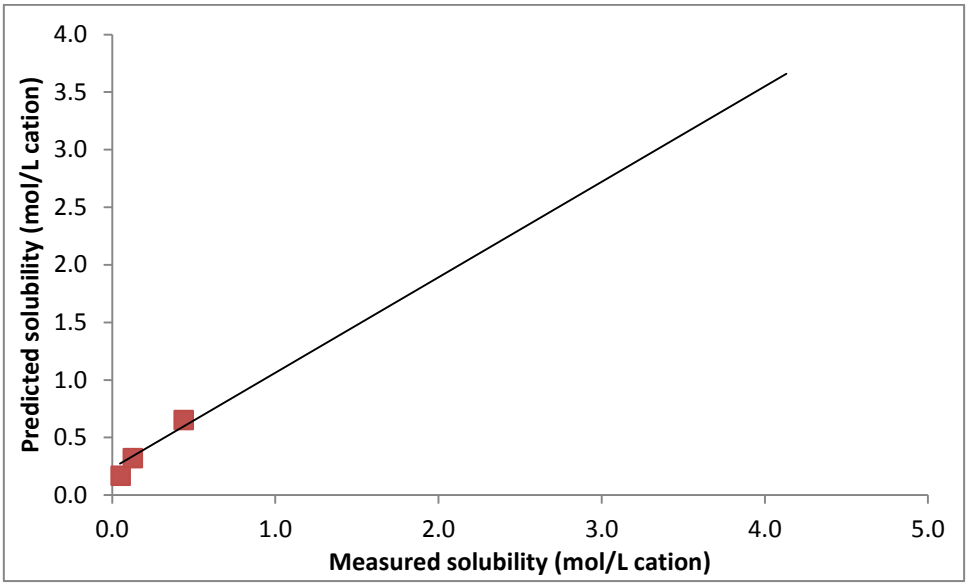

Figure D.3 Plot of measured versus predicted solubility for the uncorrected prediction test set of methylephedrinium conglomerate salts. Line obtained from training set, **red** represents methylephedrinium salts

Table D.2 Observed and predicted solubility results for the uncorrected prediction test set of methylephedrinium conglomerate salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	3	0	0	0.0

D.3.2 Predicting solubility for phenethylammonium salts using uncorrected regression and classification training sets

The uncorrected training sets have no ability to predict the solubility of the phenethylammonium salts, either using the regression or classification model, see Figure D.4 and Table D.3.

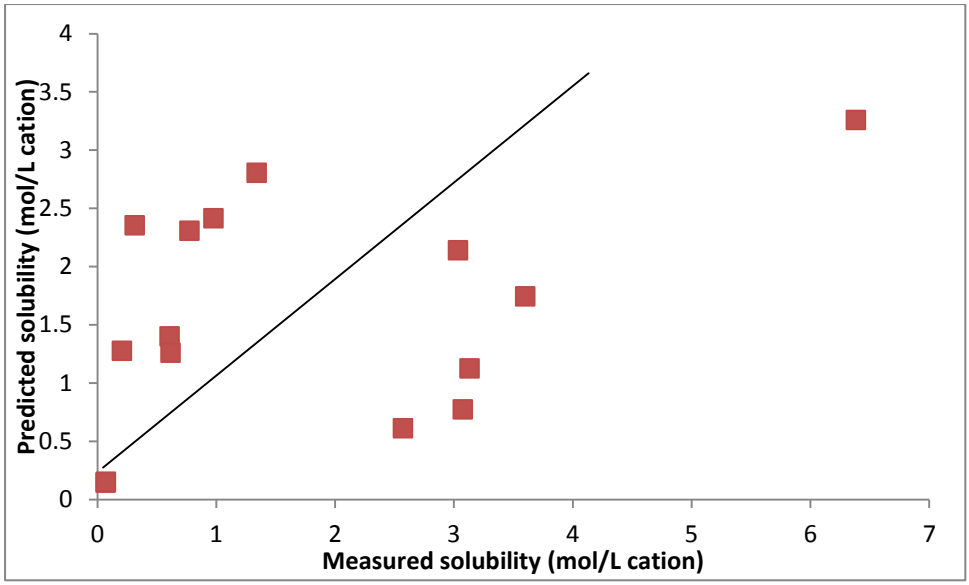

Figure D.4 Plot of measured versus predicted solubility for the uncorrected prediction test set of phenethylammonium salts. Line obtained from training set, **red** represents phenethylammonium salts

Table D.3 Observed and predicted solubility results for the uncorrected prediction test set of phenethylammonium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	2	4	0	66.6
Soluble	0	1	2	66.6
Very soluble	4	0	2	66.6

D.3.3 Predicting solubility for phenylpropylammonium salts using uncorrected regression and classification training sets

Again the uncorrected training sets have every little success in the prediction of aqueous solubility for salts of phenylpropylamine, see Figure D.5 and Table D.4.

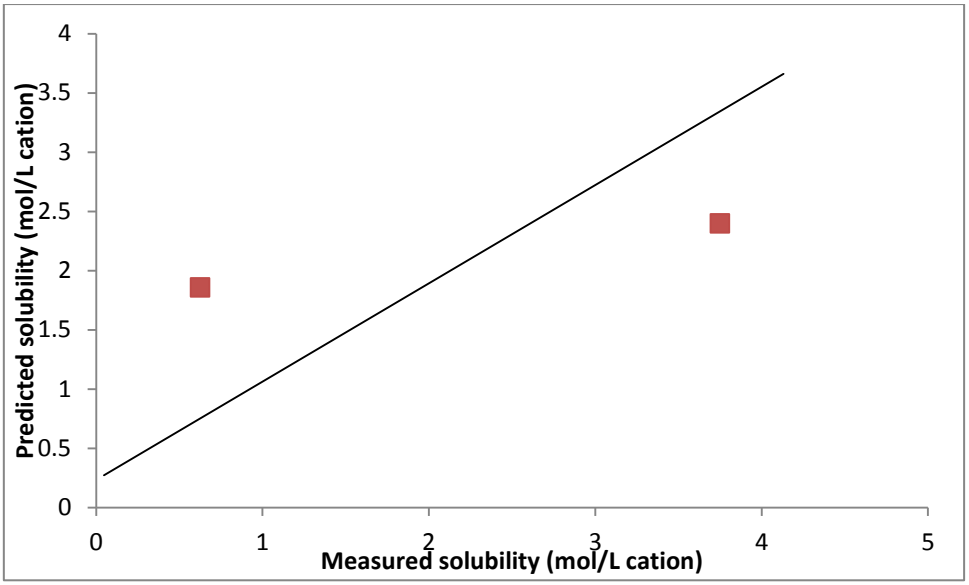

Figure D.5 Plot of measured versus predicted solubility for the uncorrected prediction test set of phenylpropylammonium salts. Line obtained from training set, **red** represents phenylpropylammonium salts

Table D.4 Observed and predicted solubility results for the uncorrected prediction test set of phenylpropylammonium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	0	1	0	100.0
Very soluble	0	0	1	0.0

D.3.4 Predicting solubility for tyrammonium salts using uncorrected regression and classification training sets

The uncorrected dataset was still unable to predict any solubility measurements using the regression model, see Figure D.6. The classification model was more successful only wrongly predicting two from twenty solubility categories, see Table D.5.

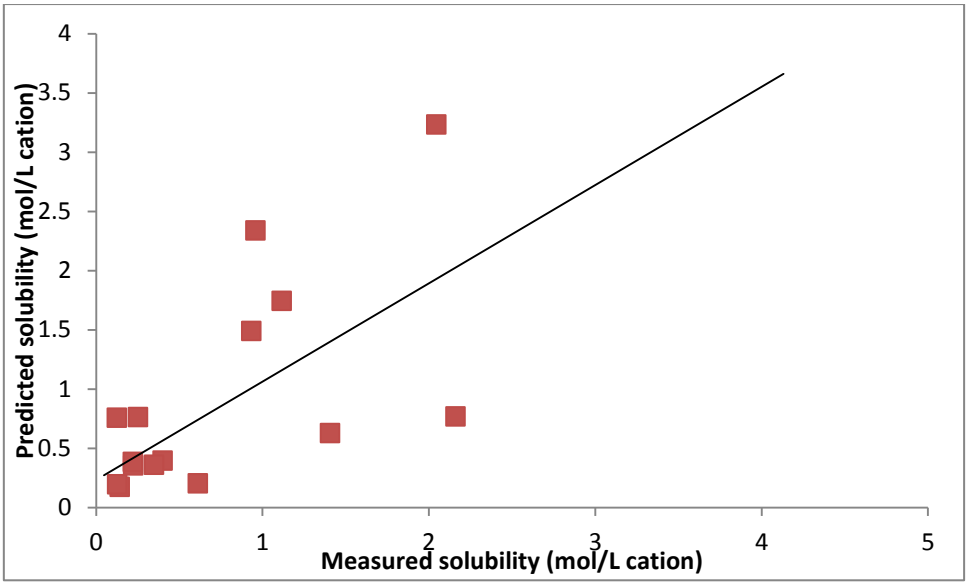

Figure D.6 Plot of measured versus predicted solubility for the uncorrected prediction test set of tyrammonium salts. Line obtained from training set, **red** represents tyrammonium salts

Table D.5 Observed and predicted solubility results for the uncorrected prediction test set of tyrammonium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	12	0	0	0.0
Soluble	1	4	0	20.0
Very soluble	1	0	2	33.3

D.3.5 Predicting solubility for methylphenethylaminium salts using uncorrected regression and classification training sets

This dataset contains ten salts of which after analysis using the classification model half of the salts were predicted into the correct solubility category, see Table D.6. The regression training set again had no consistency in prediction, see Figure D.7.

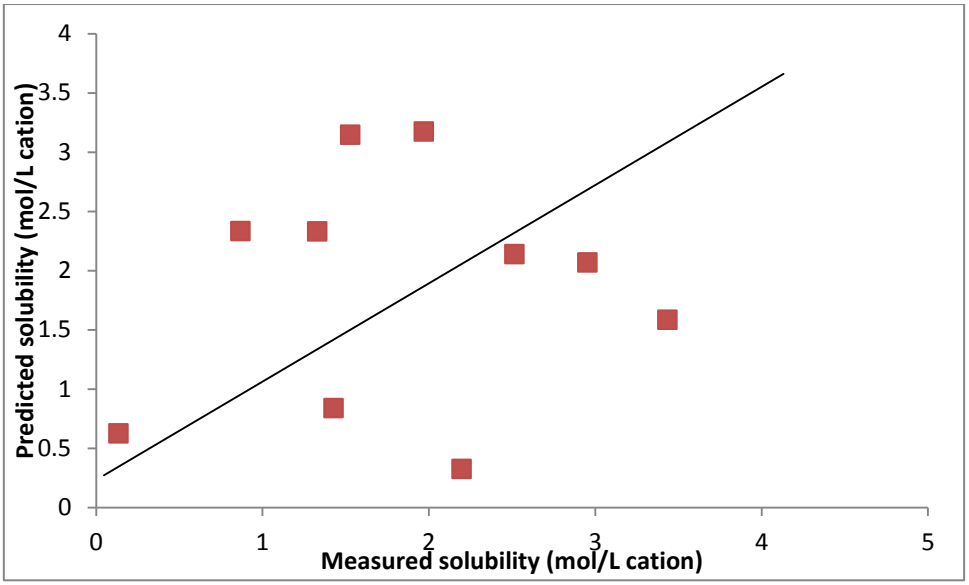

Figure D.7 Plot of measured versus predicted solubility for the uncorrected prediction test set of methylphenethylaminium salts. Line obtained from training set, **red** represents methylphenethylaminium salts

Table D.6 Observed and predicted solubility results for the prediction test set of methylphenethylaminium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	1	0	0	0.0
Soluble	1	0	3	100.0
Very soluble	0	1	4	20.0

D.3.6 Predicting solubility for α(methylaminomethyl)benzyl alcohol salts using uncorrected regression and classification training sets

This group contains eight salts of which five were correctly predicted into the right solubility category with the uncorrected classification prediction method, see Table D.7. As with the corrected training sets, the regression model appears to correctly predict the solubility of five salts, see Figure D.8.

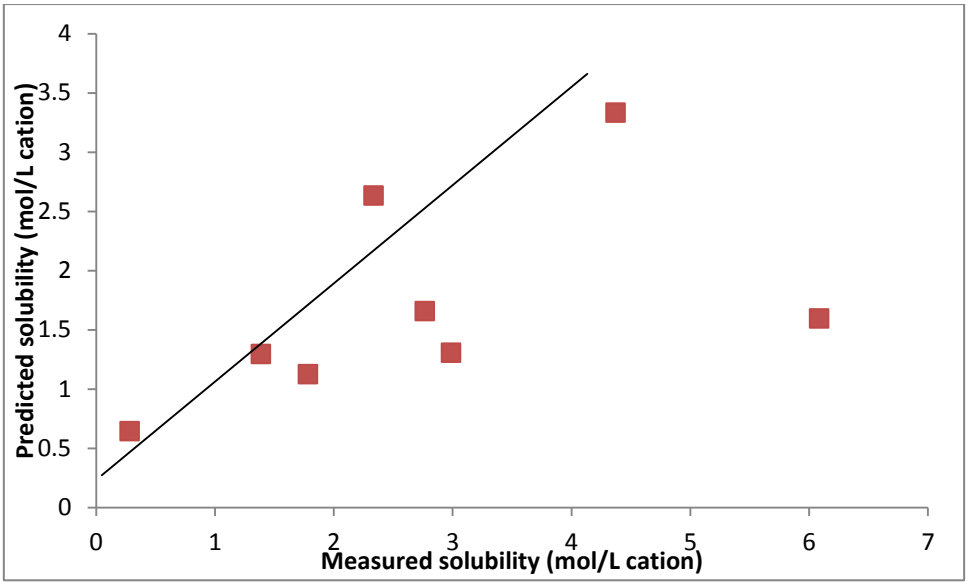

Figure D.8 Plot of measured versus predicted solubility for the uncorrected prediction test set of α(methylaminomethyl)benzyl alcohol salts. Line obtained from training set, **red** represents α(methylaminomethyl)benzyl alcohol salts

Table D.7 Observed and predicted solubility results for the uncorrected prediction test set of α(methylaminomethyl)benzyl alcohol salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	0	1	0	100.0
Soluble	0	1	0	0.00
Very soluble	1	1	4	33.3

D.3.7 Predicting solubility for (-)ephedrinium salts using uncorrected regression and classification training sets

This dataset contains fourteen salts from varying solubility categories. Although the regression model is quite erratic it appears to again predict a portion of the salts' solubility to within a reasonable error, see Figure D.9. Table D.8 shows there observed category versus their predicted category for the salts predicted using the uncorrected classification training set.

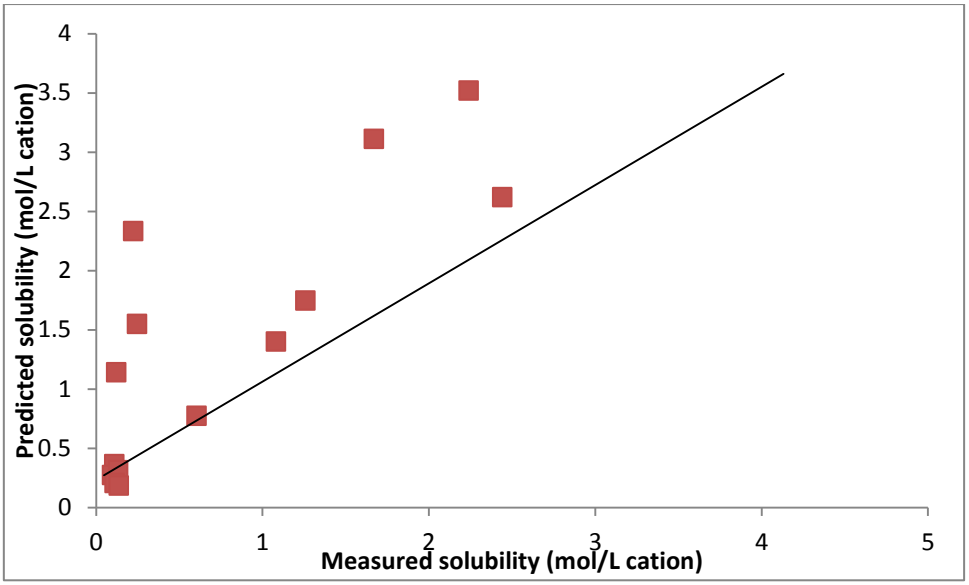

Figure D.9 Plot of measured versus predicted solubility for the uncorrected prediction test set of ephedrinium salts. Line obtained from training set, **red** represents ephedrinium salts

Table D.8 Observed and predicted solubility results for the uncorrected prediction test set of ephedrinium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	6	3	0	33.3
Soluble	0	1	2	66.6
Very soluble	1	0	1	50.0

D.3.8 Predicting solubility for (-)pseudoephedrinium salts using uncorrected regression and classification training sets

There are eight salts containing the (-)pseudoephedrine cation that were analysed. Similar to the above the regression analysis is able to reasonable predict the solubility for a portion of the salts, see Figure D.10. The classification model however has little success at correctly predicting salt solubility, see

Table D.9.

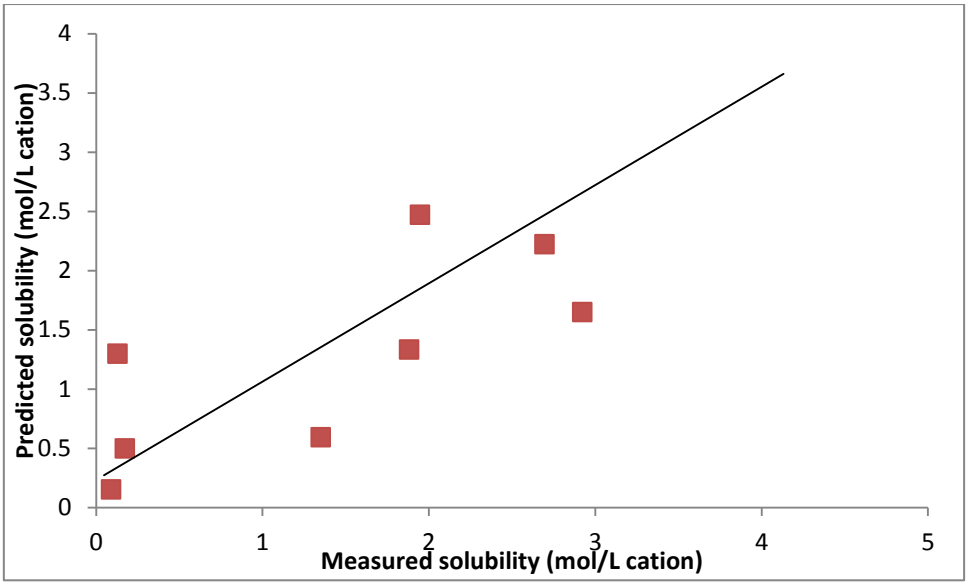

Figure D.10 Plot of measured versus predicted solubility for the uncorrected prediction test set of pseudoephedrinium salts. Line obtained from training set, **red** represents psuedoephedrinium salts

Table D.9 Observed and predicted solubility results for the uncorrected prediction test set of pseudoephedrinium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	1	2	0	66.6
Soluble	1	0	0	100.0
Very soluble	0	1	3	25.0

D.3.9 Predicting solubility for dimethylphenethylaminium salts using uncorrected regression and classification training sets

The final dataset to be examined was that of the five dimethylphenethylaminium salts, the results are shown below in Figure D.11 and Table D.10. The regression model and the classification model were able to successfully predict the solubility without too much associated error.

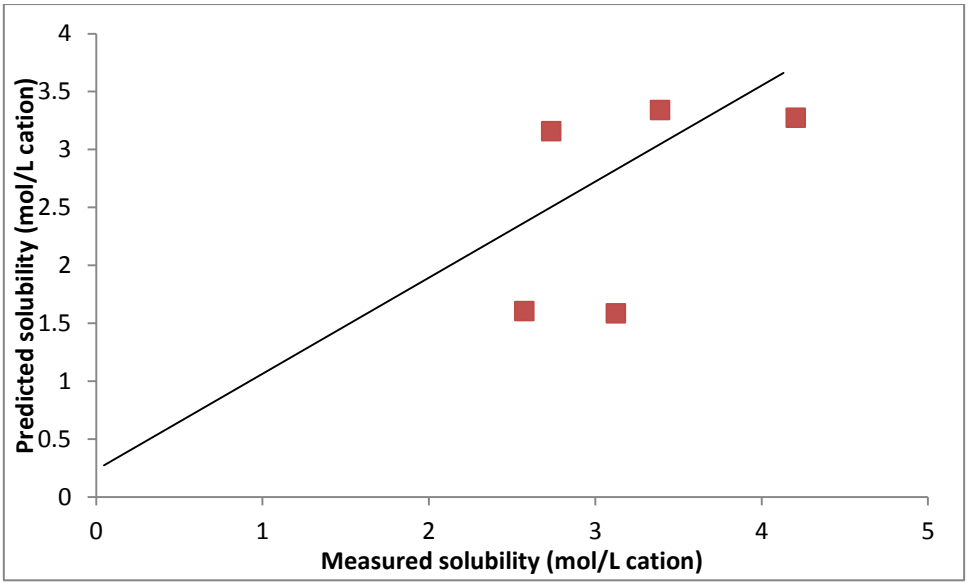

Figure D.11 Plot of measured versus predicted solubility for the uncorrected prediction test set of dimethylphenethylaminium salts. Line obtained from training set, **red** represents dimethylphenethylaminium salts

Table D.10 Observed and predicted solubility results for the uncorrected prediction test set of dimethylphenethylaminium salts

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Very soluble	0	1	4	20.0

D.3.10 Summary of success of using uncorrected training sets to predict solubility of salts from various cations

In comparison to the corrected models the results obtained here are not as good at predicting aqueous solubility. The summary of the classification model is shown below in D.11, here it is apparent the increased errors seen with this model.

Table D.11 Observed and predicted solubility results for the entire test set using uncorrected parameters

Predicted → / Observed ↓	Sparingly soluble	Soluble	Very soluble	Prediction error (%)
Sparingly soluble	26	10	0	27.8
Soluble	3	7	7	58.8
Very soluble	8	3	21	34.4

D.4 Appendix references

(1) Rademeyer, M. *Acta Crystallographica Section E-Structure Reports Online* **2007**, *63*, O221.
(2) Horn, E.; Tiekink, E. R. T.; Jones, G. P.; Naiola, B. P.; Paleg, L. G. *Acta Crystallographica Section C-Crystal Structure Communications* **1990**, *46*, 1575.
(3) Haynes, D. A.; Pietersen, L. K. *Crystengcomm* **2008**, *10*, 518.
(4) Barlow, R. B.; Johnson, O.; Howard, J. A. K.; Walton, D. C.; Koellner, G. *Acta Crystallographica Section B-Structural Science* **1989**, *45*, 396.
(5) Koleva, B. B.; Kolev, T.; Seidel, R. W.; Spiteller, M.; Mayer-Figge, H.; Sheldrick, W. S. *J. Mol. Struct.* **2008**, *888*, 138.
(6) Collier, E. A.; Davey, R. J.; Black, S. N.; Roberts, R. J. *Acta. Cryst.* **2006**, *A62*, 498.
(7) Bergin, R. *Acta Crystallographica Section B-Structural Crystallography and Crystal Chemistry* **1971**, *B 27*, 381.
(8) Hearn, R. A.; Bugg, C. E. *Acta Crystallographica Section B-Structural Science* **1972**, *28*, 3662.
(9) Hearn, R. A.; Freeman, G. R.; Bugg, C. E. *J. Am. Chem. Soc.* **1973**, *95*, 7150.
(10) Mathew, M.; Palenik, G. J. *Acta Crystallographica Section B-Structural Science* **1977**, *33*, 1016.
(11) Duddu, S. P.; Grant, D. J. W. *Pharm. Res.* **1994**, *11*, 1549.