

Electronic Supplementary Information†

Crystal structures of Mirtazapine molecular salts†

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Table S1 Rietveld refinement parameters for overlay of experimental and calculated XRD lines.

	Mirtazapine hemihydrate	Mirtazapinium hydrogenmalonate	Mirtazapinium hydrogenmaleate	Mirtazapinium hemidiadipate	Mirtazapinium hydrogenfumarate monohydrate	Mirtazapinium salicylate
Rp	8.88	9.32	8.15	11.21	8.00	8.16
Rwp	13.10	12.51	11.64	15.69	10.43	10.87
scaling	Old: 2.6751 New: 2.6751	Old: 3.4492 New: 3.4492	Old: 2.5206 New: 2.5206	Old: 3.4190 New: 3.4190	Old: 1.7817 New: 1.7817	Old: 2.9399 New: 2.9399
lattice	Old: a = 9.8081 b = 17.3256 c = 9.0160 β = 106.0591	Old: a = 10.3359 b = 10.8052 c = 10.8930 α = 111.0824 β = 115.9434 γ = 99.6507	Old: a = 8.9356 b = 9.8959 c = 22.4951	Old: a = 10.6832 b = 9.3652 c = 18.1492 β = 103.1928	Old: a = 25.2977 b = 18.5764 c = 8.8859 β = 102.7990	Old: a = 13.9468 b = 15.6265 c = 9.4503 β = 99.7808

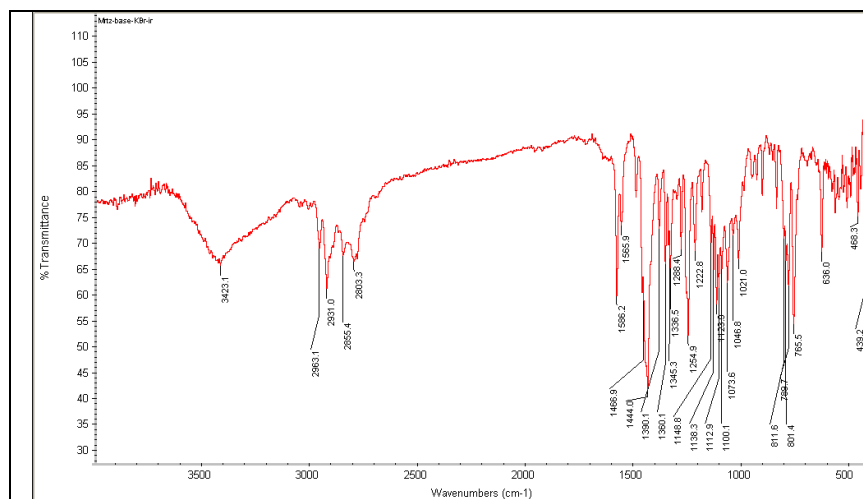
	New: a = 9.8081 b = 17.3256 c = 9.0160 β = 106.0591	New: a = 10.3359 b = 10.8052 c = 10.8930 α = 111.0824 β = 115.9434 γ = 99.6507	New: a = 8.9356 b = 9.8959 c = 22.4951	New: a = 10.6832 b = 9.3652 c = 18.1492 β = 103.1928	New: a = 25.2977 b = 18.5764 c = 8.8859 β = 102.7990	New: a = 13.9468 b = 15.6265 c = 9.4503 β = 99.7808
profile U	Old: -0.1805	0.0619	0.0732	0.5000	-0.3166	-0.4900
	New: -0.1805	0.0618	0.0732	0.5000	-0.3166	-0.4900
PsVoigt2	Old: V = 0.0000	0.0000	0.0000	0.0008	0.0000	0.0000
	New: V = 0.0000	0.0000	0.0000	0.0008	0.0000	0.0000
	Old: W = 0.1566	0.1461	0.1408	0.1723	0.1520	0.1721
	New: W = 0.1566	0.1461	0.1408	0.1723	0.1520	0.1721
overall B	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table S2 FT-IR (KBr pellet) and FT-Raman (neat solid) spectral bands of Mirtazapine salts.

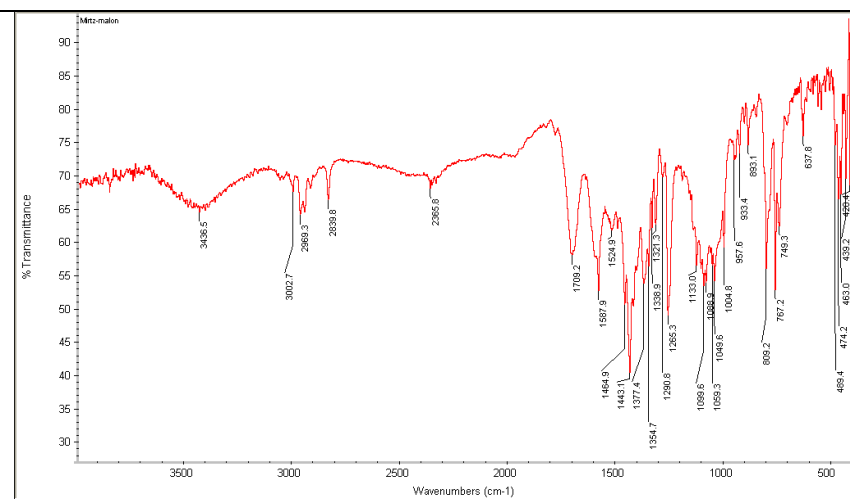
	Mirtazapine hemihydrate	Mirtazapinium hydrogenmalonate	Mirtazapinium hydrogenmaleate	Mirtazapinium hemiadipate ^a	Mirtazapinium hydrogenfumarate monohydrate	Mirtazapinium salicylate	Mirtazapinium diHCl trihydrate
FT-IR bands							
O–H stretching	3423 br (water)	3436 br (acid)	3414 br (acid)	3424 br (acid)	3439 br (acid, water)	3427 br (acid)	3430, 3382 br (water)
N–H stretching	---	3436 br (merged)	3414 br (merged)	3424 br (merged)	3439 br (merged)	3427 br (merged)	3430, 3382 br (merged)
N–H bend	---	1443	1443	1428	1440	1444	1443
COO [−] (C=O)	---	1709 (acid)	1697 (acid)	1696 (acid)	1697 (acid)	1641 (acid)	---
C–H stretch (CH ₃ group)	2963, 2931	2969	2960	2945, 2918	2951, 2922	2974, 2923	2979, 2964
pyridine ring stretch	1586, 1566, 1467 and 1444	1588, 1525, 1465 and 1443	1618, 1578, 1455 and 1443	1593, 1576, 1460 and 1445	1589, 1573, 1459 and 1440	1588, 1570, 1488 and 1456	1620, 1599, 1537 and 1444
FT-Raman bands							
O–H stretching	---			---	3444	3437	3443
N–H stretching	3059, 3044	3076, 3048	3068, 3040	---	3052, 3041	3062,	3059
N–H bend	2964	2972, 2950	2999, 2960	---	2979, 2952	2975, 2946	2980, 2949
COO [−] (C=O)	---	1603 (merged)	1706	---	1707	1602 (merged)	---
C–H stretch (CH ₃ group)	2933, 2905	2920, 2907	2900, 2862	---	2890, 2855	2888, 2846	2914, 2854

pyridine ring stretch	1604, 1585, 1461, 1440	1603, 1587, 1457, 1429	1601, 1582, 1457, 1438	---	1602, 1586, 1459, 1431	1602, 1584, 1455, 1434	1599, 1582, 1461, 1440
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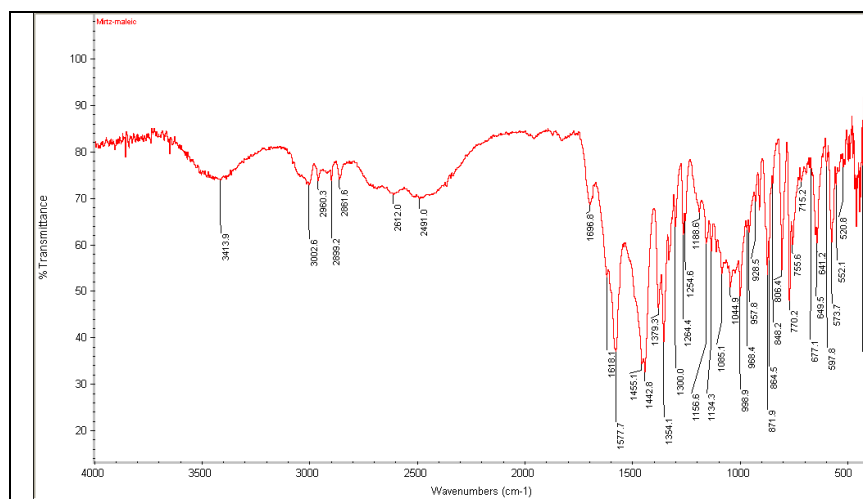
^a Raman spectrum could not be recorded of Mirtazapine hemiadipate because the sample suffered charring due to laser radiation



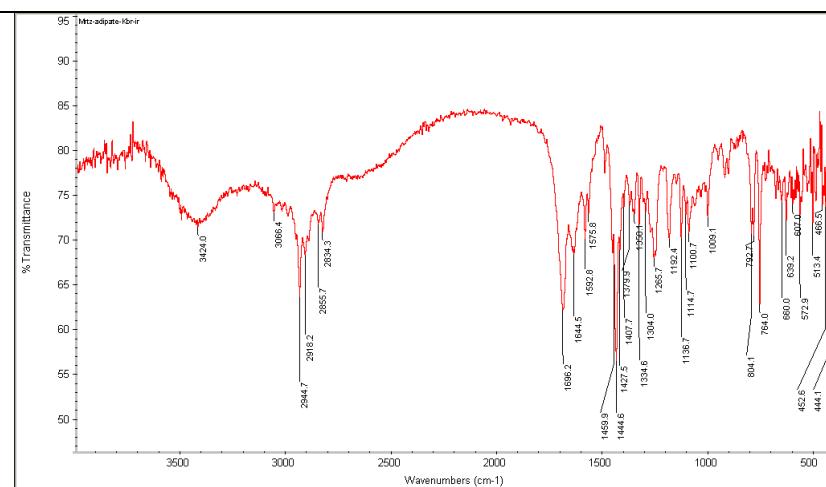
FT-IR Mirtazapine hemihydrate



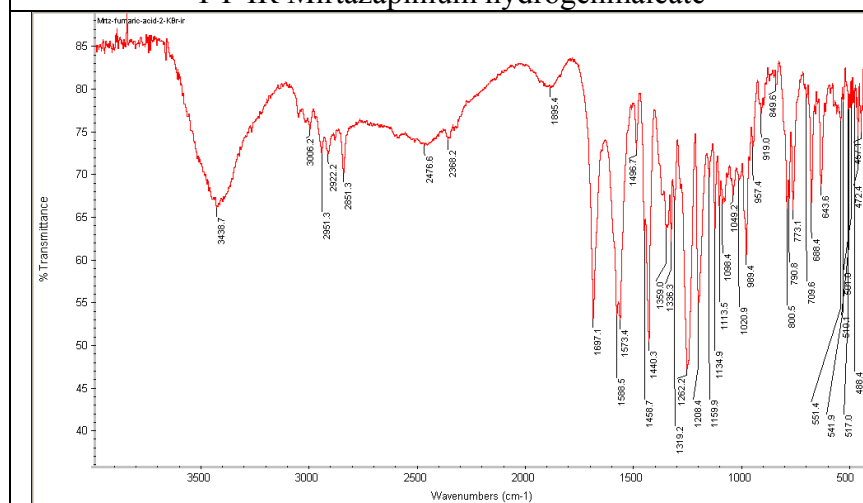
FT-IR Mirtazapine hydrogenmalonate



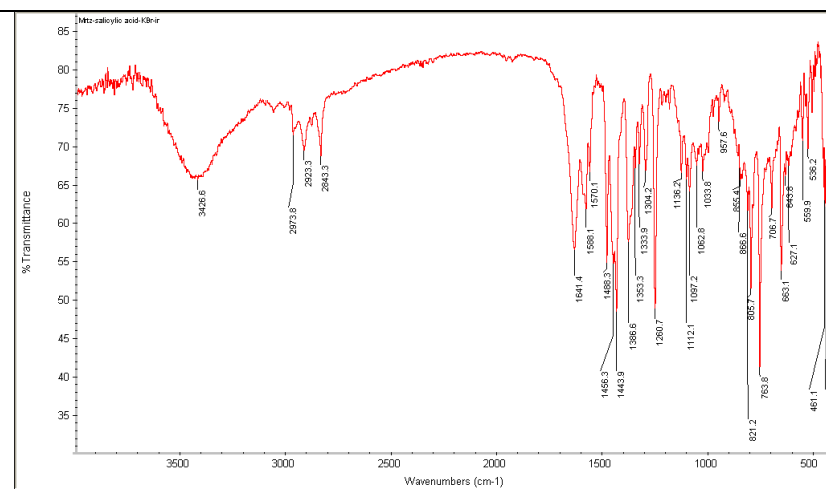
FT-IR Mirtazapinium hydrogenmaleate



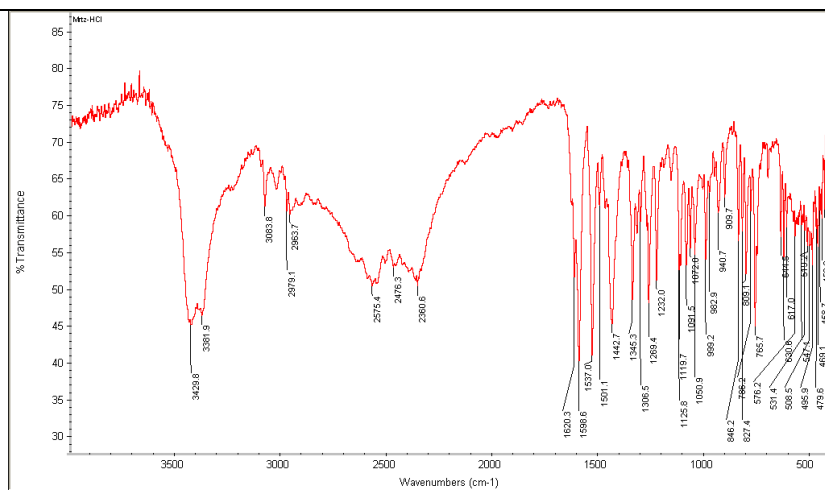
FT-IR Mirtazapinium hemiadipate



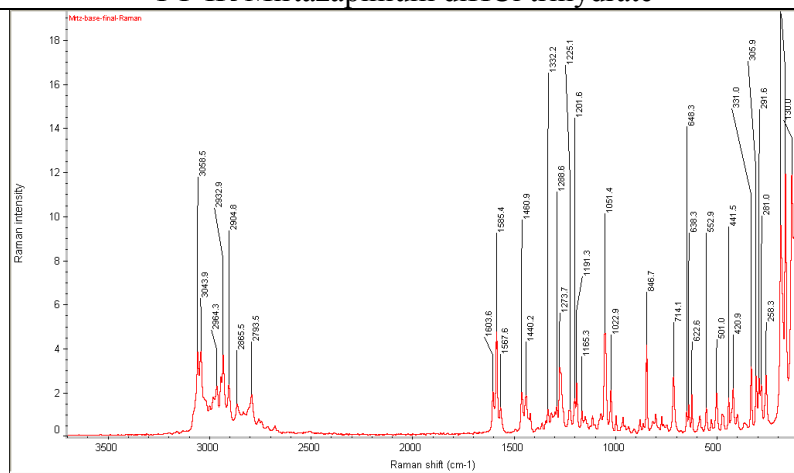
FT-IR Mirtazapinium hydrogenfumarate monohydrate



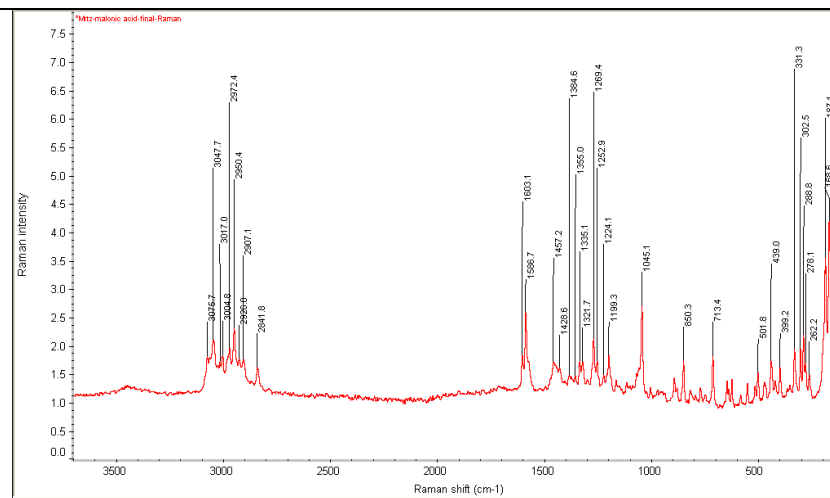
FT-IR Mirtazapinium salicylate



FT-IR Mirtazapine diHCl trihydrate



FT-Raman Mirtazapine hemihydrate



FT-Raman Mirtazapine hydrogenmalonate

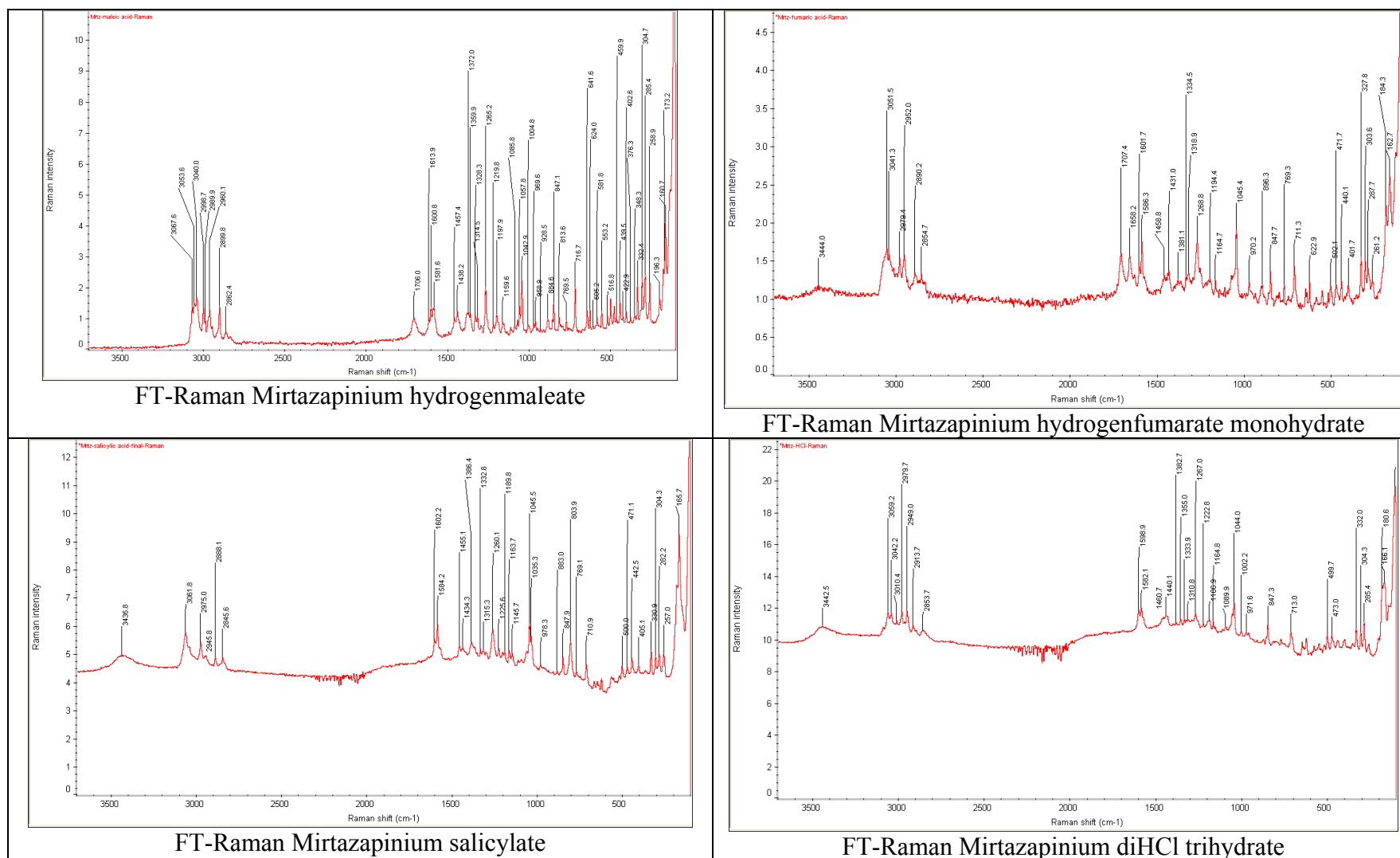
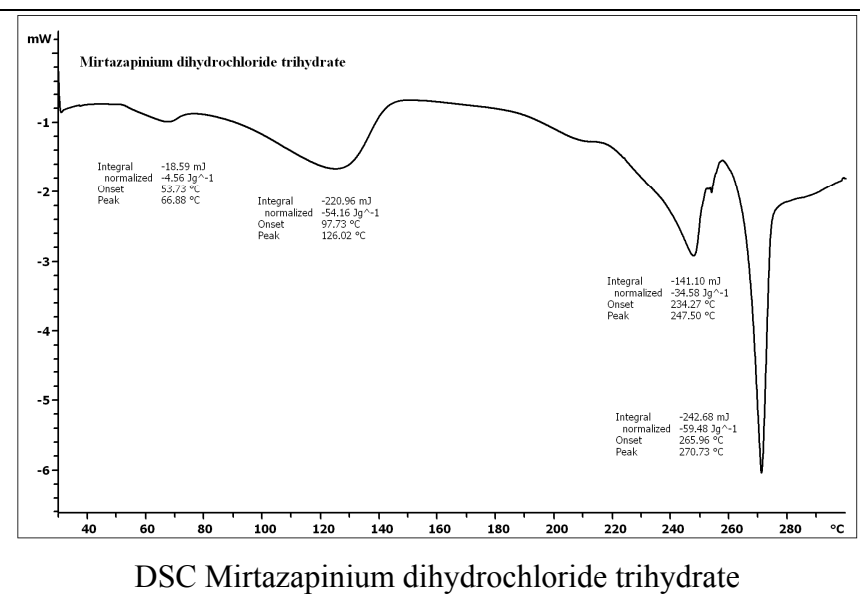
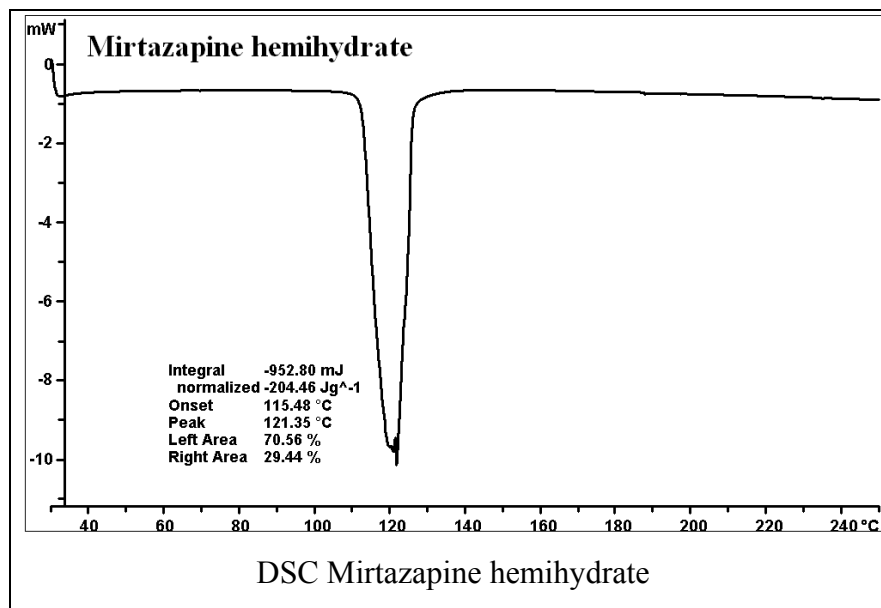
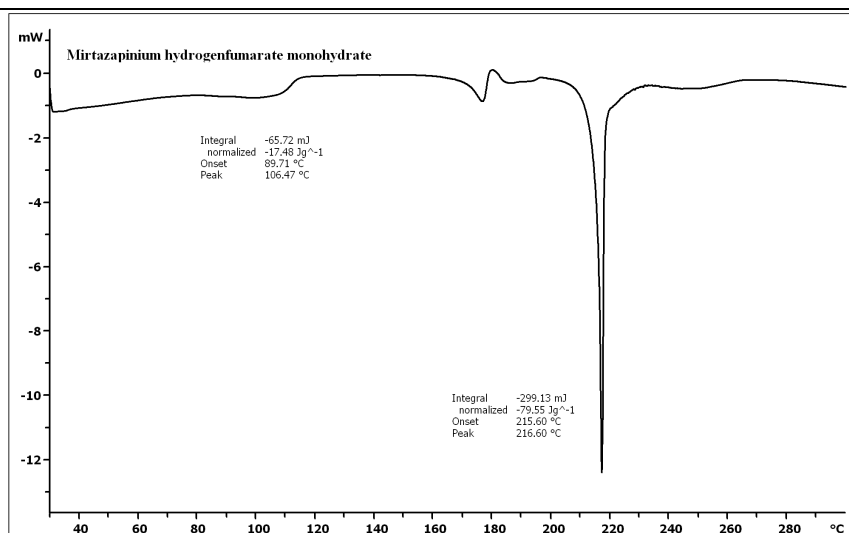
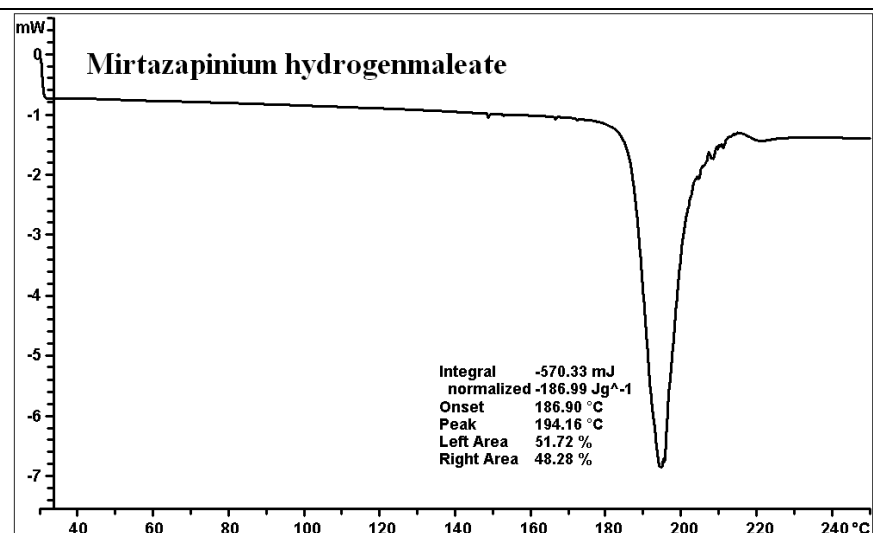


Figure S1 IR and Raman spectra of Mirtazapine salts. The Raman spectrum of Mirtazapinium hemiadipate could not be recorded because of sample charring by the laser.

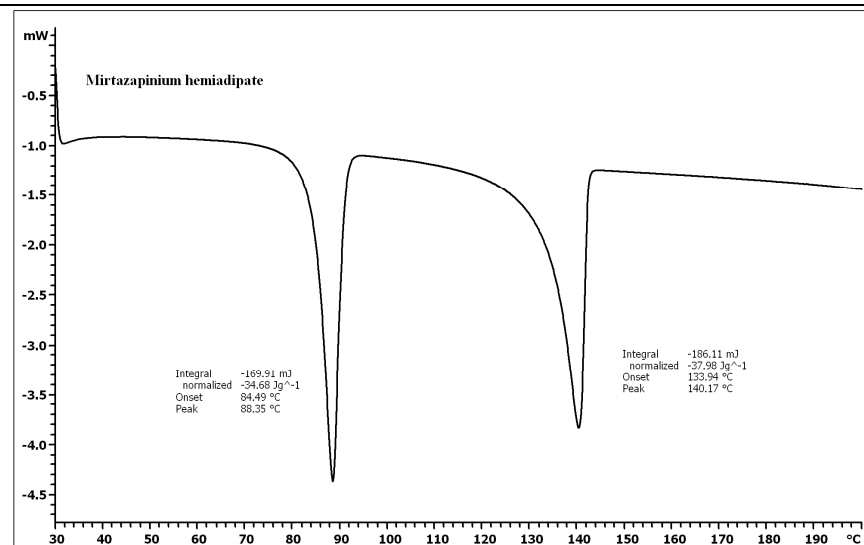
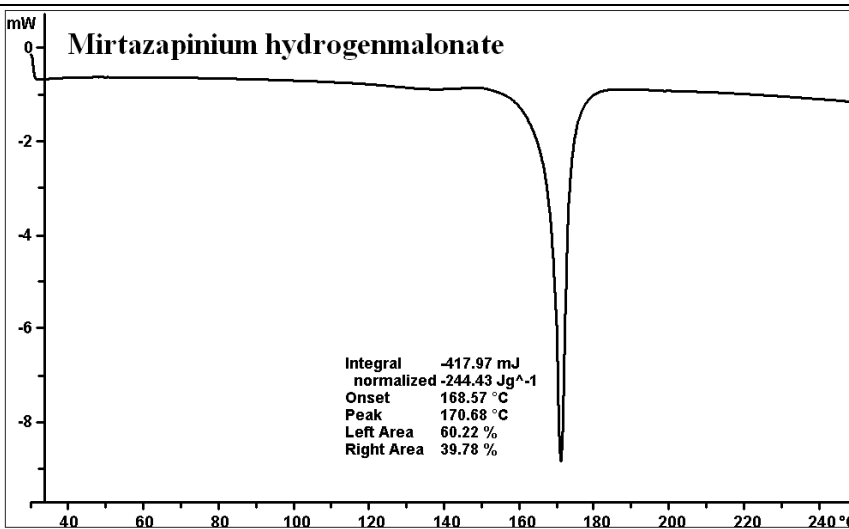


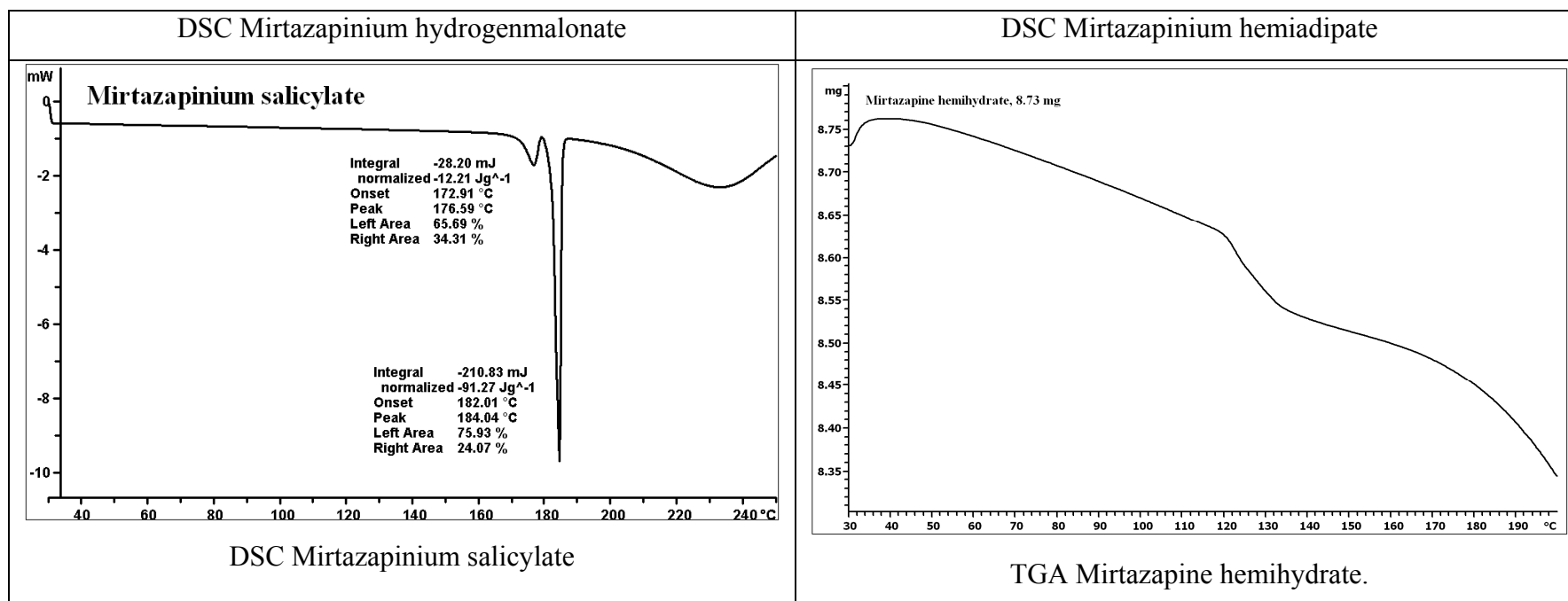


DSC Mirtazapinium hydrogenfumarate monohydrate



DSC Mirtazapinium hydrogenmaleate





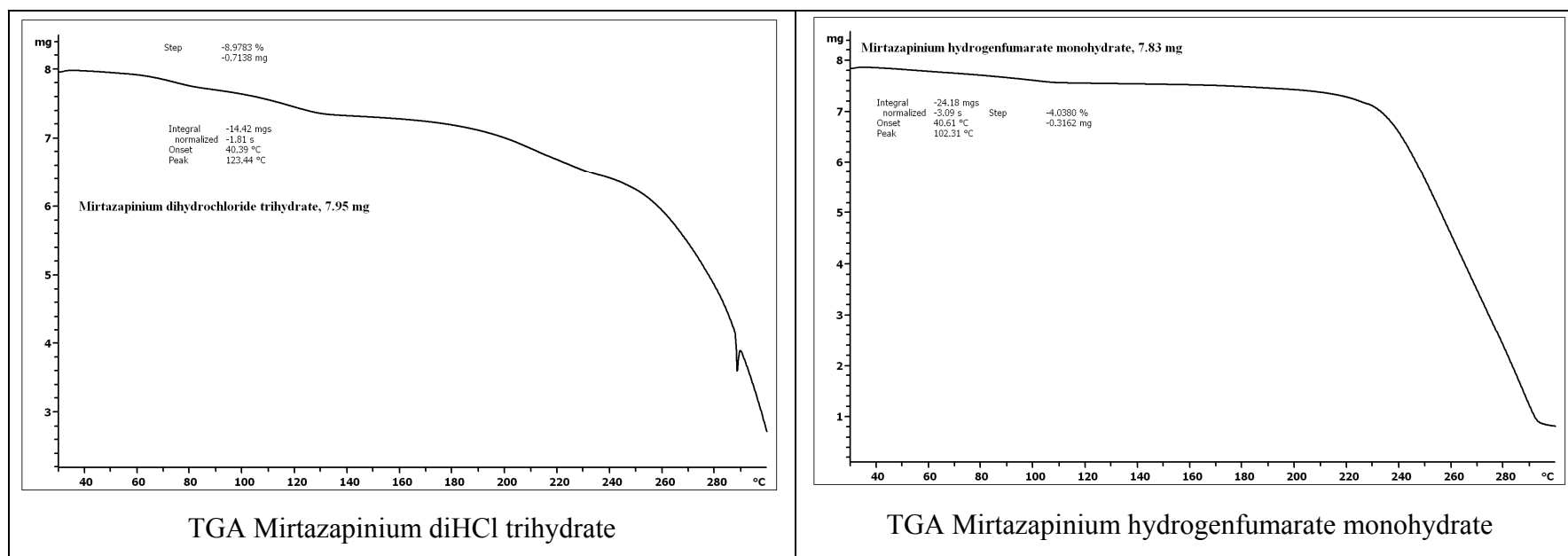


Figure S2 DSC and TGA of Mirtazapine salts.

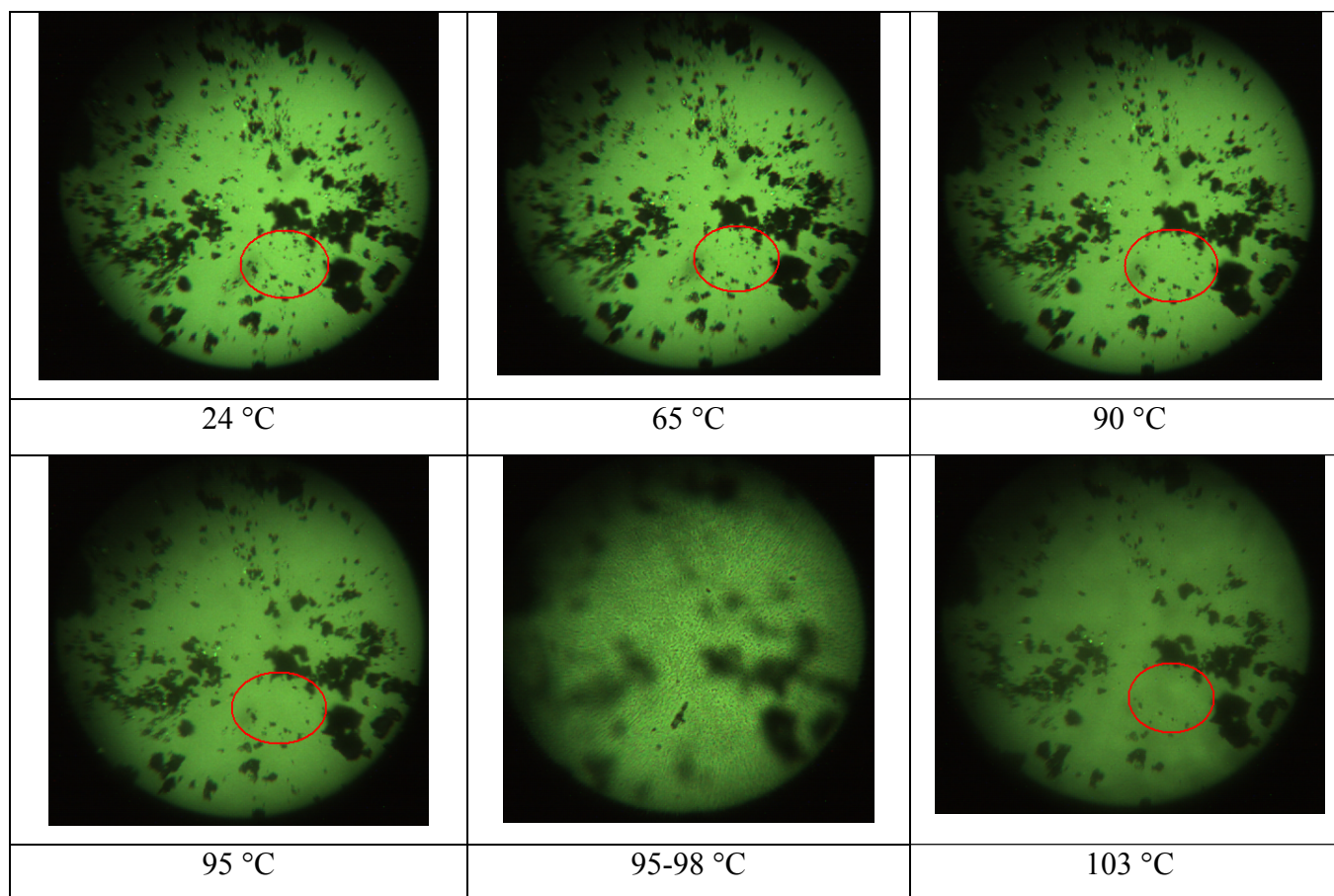




Figure S3 HSM snapshots of Mirtazapine hemihydrate. The solid in the red circle starts to disappear with heating and makes a cloudy deposition on the glass slide at 95 °C and is melted by 110 °C. Our visual observation suggests that sublimation begins around 65 °C and melting occurs at 110 °C. The glass lid is covered with the sublimed material at 95-98 °C.