Combinatorial library approach to realize 2-aminothiazole based two components gelator: A structure-property correlation

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Supporting Information

Analytical data

Compound-B1A1. m.p 146 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ7.793(s, 2H, NH_2), 7.072(d, 1H, CH), 6.697(d, 1H, CH), 6.168(d, 2H, CH=CH).

FT-IR(KBr pellet); 3239,3123,2311,1908,1701,1684,1616,1519,1355,1212,1168,1036, 980,788,711,611,499,415.

Compound-B1A2. m.p 174 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ7.701(s, 2H, NH_2), 6.986(d, 1H, CH), 6.920(d, 1H, CH), 6.605(d, 2H, CH=CH).

FT-IR(KBr pellet); 3210,3165,2218,1928,1817,1704,1669,1613,1559,1372,1210,1143,1080, 1018,918,816,788,711,668,558,450,415.

Compound- B1A3. m.p 105 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ7.197(s, 2H, NH_2), 6.942 (d, 1H, CH), 6.595(d, 1H, CH), 3.195(s, 2H, CH_2).

FT-IR(KBr pellet); 3169,3086,2748,1908,1743,1685,1625,1580,1467,1410,1268 , 1220, 1168,987,866, 746,606,563,502,440.

Compound-B1A4. m.p 69 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ 6.896(s, 2H, NH_2), 6.833 (d, 1H, CH), 6.545(d, 1H, CH), 2.201(t, 4H, CH_2), 1.477-1.443(m, 4H, CH_2).

FT-IR(KBr pellet);3495,3366,3127,2484,1930,1699,1658,1634,1567,1519,1456,1327, 1315, 1279,1198,1166,1014,925,901,793,710,563,538,485,418.

Compound-B1A5. m.p 78 ^{0}C, ^{1}HNMR (400MHZ, MEOD, TMS); δ6.917 (d, 1H, CH), 6.576(d, 1H, CH), 2.332-2.285(t, 4H, CH_2), 1.663-1.590(m, 4H, CH_2), 1.399-1.381(m, 4H, CH_2).

FT-IR(KBr pellet);3390,3197,2930,2355,1700,1632,1512,1467,1411,1349,1255,1191, 1052, 930,795,726,684,560,499.

Compound-B1A6. m.p 104 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.947(s, 2H, NH_2), 6.887(d, 1H, CH), 6.543(d, 1H, CH), 2.111-2.150(t, 4H, CH_2), 1.490-1.456(m, 4H, CH_2), 1.291-1.240 (m, 4H, CH_2).

FT-IR(KBr pellet);3381,3196,2936,2363,1699,1634,1509,1467,1408,1354,1299,1239, 1187, 1051,931,860,723,680,543,415.

Compound-B1A6a. m.p 97^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.864(s, 4H, NH_2), 6.914(d, 2H, CH), 6.527(d, 2H, CH), 2.196-2.160(t, 4H, CH_2), 1.493-1.458(m, 4H, CH_2), 1.296-1.243 (m, 4H, CH_2).

FT-IR(KBr pellet); 3270,3262389,1840,1714,1653,1619,1592,1484,1361,1301,1229,1132, 980,852,784,665,589,496,423

Compound-B1A7. m.p 88 ^{0}C, ^{1}HNMR (400MHZ, MEOD, TMS); δ6.970 (d, 1H, CH), 6.574(d, 1H, CH), 2.311-2.274(t, 4H, CH_2), 1.631-1.577(m, 4H, CH_2), 1.355-1.308(m, 4H, CH_2).

FT-IR(KBr pellet);3390,3193,2852,2460,1913,1699,1628,1506,1467,1407,1342,1277, 1185, 1060,931,902,864,722,686,532,474.

Compound-B2A1. m.p 138 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ8.088(s, 2H, NH_2), 6.318(d, 1H, CH), 6.147(s, 2H, CH=CH), 2.107(d, 3H, CH_3).

FT-IR(KBr pellet);3320,3103,2504,1880,1704,1655,1625,1584,1464,1355,1209,1072,982, 943,784,65,586,528,423

Compound-B2A2. m.p 148 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.8598(s, 2H, NH_2), 6.620(s, 2H, CH=CH), 6.085(d, 1H, CH), 2.049(d, 3H, CH_3).

FT-IR(KBr pellet);3125,2328,1914,1792,1711,1667,1642,1562,1519,1429,1371,1275, 1200, 1163,979,825,800,712,579,432.

Compound-B2A3. m.p 133 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.932(s, 2H, NH_2), 6.105(d, 1H, CH), 3.208(s, 2H, CH2), 2.055(d, 3H, CH_3)

FT-IR(KBr pellet);3296,3130,2488,1920,1714,1667,1606,1455,1361,1271,1189,1025,948, 891,824,750,504,539,456.

Compound-B2A4. m.p103 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.787 (s, 2H, NH_2), 6.076 (d, 1H, CH), 2.216-2.187(t, 4H, CH_2), 2.046(d, 3H, CH_3), 1.502-1.480(m, 4H, CH_2).

FT-IR(KBr pellet);3234,2939,1793,1712,1639,1600,1536,1409,1350,1319,1250,1175,923, 888,728,620,591,523,439.

Compound-B2A5. m.p 99 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.790 (d, 2H, NH_2), 6.076 (d, 1H, CH), 2.202-2.165(t, 4H, CH_2), 2.047(d, 3H, CH_3), 1.489-1.453(m, 4H, CH_2), 1.268-1.250(m, 4H, CH_2).

FT-IR(KBr pellet);3427,3052,2936,2528,1932,1684,1614,1542,1465,1352,1253,1156, 1102, 1007,932,725,684,565,491.

Compound-B2A6. m.p 89 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.744 (s, 2H, NH_2), 6.086 (d, 1H, CH), 2.017(d, 3H, CH_3)2.178-2.142(t, 4H, CH_2), 1.455-1.421(m, 4H, CH_2), 1.220-1.196(m, 8H, CH_2).

FT-IR(KBr pellet);3402,3296,2406,1937,1709,1622,1525,1469,1431,1366,1299,1237, 1186, 1117,1045,985,898,768,676,543,426.

Compound-B2A6a. m.p 84^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.842 (s, 4H, NH_2), 6.145 (d, 2H, CH), 2.232(d, 6H, CH_3), 2.170-2.153(t, 4H, CH_2), 1.420-1.409(m, 4H, CH_2), 1.238-1.209(m, 8H, CH_2).

FT-IR(KBr pellet);3306,2506,1897,1714,1632,1565,1453,1399,1366,1239,1217,1146, 1107, 1023,965,802,752,626,523,465,436.

Compound-B2A7. m.p 92 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.768 (s, 2H, NH_2), 6.074 (d, 1H, CH), 2.049(d, 3H, CH_3), 2.197-2.160(t, 4H, CH_2), 1.491-1.456(m, 4H, CH_2), 1.220-1.196(m, 12H, CH_2).

FT-IR(KBr pellet);3404,3114,2526,1942,1802,1712,1653,1522,1422,1302,1226,1116, 925, 797,720,680,520,432.

Compound-B3A1. m.p 142 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ7.957(s, 2H, NH_2), 6.826(d, 1H, CH), 6.142(s, 2H, CH=CH), 2.203(d, 3H, CH_3)

FT-IR(KBr pellet); 3423,3075,2719,1899,1704,1662,1616,1567,1470,1359,1256,1208, 1180, 1041,923,877,819,753,638,600,504,421.

Compound-B3A2. m.p 182 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.700(s, 2H, NH_2), 6.620(s, 2H, CH=CH), 6.577(d, 1H, CH), 2.172(d, 3H, CH_3).

FT-IR(KBr pellet);3325,3031,1861,1712,1684,1646,1572,1532,1430,1355,1292,1171, 1066, 996,922,824,752,705,630,560,506,413

Compound-B2A3. m.p 116 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.874(s, 2H, NH_2), 6.611(d, 1H, CH), 3.198(s, 2H, CH_2), 2.175(d, 3H, CH_3)

FT-IR(KBr pellet);3285,3129,2460,1909,1726,1682,1592,1523,1463,1340,1267,1163, 1106, 951,825,747,701,604,503,458.

Compound-B3A4. m.p 128 ^{0}C,^{1}HNMR (400MHZ, DMSO, TMS); δ6.645(s, 2H, NH_2), 6.569 (d, 1H, CH), 2.202(d, 3H, CH3), 2.184-2.166(t, 4H, CH2), 1.490-1.436(m, 4H, CH2).

FT-IR(KBr pellet);3400,3209,2947,2361,1946,1697,1634,1532,1462,1409,1357, 1277,1201, 1064,910,823,735,660,575,452.

Compound-B3A5. m.p 138 ^{0}C, ^{1}HNMR (400MHZ, DMSO, TMS); δ6.643(s, 2H, NH_2), 6.569 (d, 1H, CH), 2.227-2.218(t, 4H, CH_2), 2.203(d, 3H, CH_3), 1.523-1.505(m, 4H, CH_2), 1.268-1.250(m, 4H, CH_2).

FT-IR(KBr pellet);3057,2354,1908,1699,1643,1550,1416,1333,1255,1178,1069,854,805, 704,642,526,442,413.

Compound-B3A6. m.p 83 ^{0}C,^{1}HNMR (400MHZ, DMSO, TMS); δ6.631 (d, 2H, NH_2), 6.562 (d, 1H, CH), 2.169(d, 3H, CH_3), 2.160-2.152(t, 4H, CH_2), 1.468-1.455(m, 4H, CH_2), 1.236-1.220(m, 8H, CH_2).

FT-IR(KBr pellet);3247,2353,1888,1712,1657,1613,1536,1467,1415,1345,1308,1273,1152, 1210,1177,1064,963,874,824,755,701,643,502,427.

Compound-B3A6a. m.p 107 ^{0}C,^{1}HNMR (400MHZ, DMSO, TMS); δ6.622 (d, 4H, NH_2), 6.569 (d, 2H, CH), 2.182(d, 6H, CH_3), 2.174-2.171(t, 4H, CH_2), 1.494-1.459(m, 4H, CH_2), 1.243-1.229(m, 8H, CH_2).

FT-IR (KBr pellet);3353,3046,2917,2356,1909,1700,1667,1635,1575,1457,1371,1306, 1234, 1187,859,732,689,547,436.

Compound-B3A7. m.p 110^{0}C, ^{1}HNMR (400MHZ, MEOD, TMS); δ6.612 (d, 1H, CH), 2.307-2.269(t, 4H, CH_2), 2.255(s, 3H, CH_3), 1.631-1.595(m, 4H, CH_2), 1.335-1.220(m, 12H,CH_2).

FT-IR(KBr pellet);3422,2921,1700,1613,1469,1433,1334,1281,1226,1186,1065,929,902, 822,723,679,524,474,411.

Table S1: a) List of compounds obtained after CSD search of 2-aminothiazole based organic salts/ cocrystals

S. No.	Name of the Compounds CSD REFCODE	Supramolecular Synthon (graph set representation)	weak secondary non-covalent interactions and overall Supramolecular assembly	References
i	2-Aminothiazolium 3,5-dinitrobenzoate JEFLEM	$R_2^2(8), R_4^2(8)$	(Nitro)O....S(thiazole), 3D	Mohamed, H.A.; El-Medani, S.M.; Ramadan,R. M. *J.Indian Chem.Soc.* **2005**, 82,799.
ii	2,2'-Diamino-4,4'-bi-1,3-thiazolium fumarate TADRUM	$R_2^2(8)$	(COOH)O...S(thiazole), N-H...O, 3D	Liu,J-G.; Xu,D-J.; Sun,W-L. *Acta Crystallogr., Sect.E: Struct. Rep. Online* **2003,**59**,** o812
iii	2,2'-Diamino-4,4'-bi-1,3-thiazolium (2R,3R)-tartrate FIWJIF	$R_2^2(8)$	(COOH)O-H...O^- (COO^-), (thiazole) S...O(COOH) ,3D	Liu,B.-X.; Xu,D.J.*Acta Crystallogr., Sect.E: Struct.Rep. Online* **2005**,61**,** o753
iv	2,2'-diamino-4,4'-bi-1,3-thiazol-3,3'-diium bis(2,2'-diamino-4,4'-bi-1,3-thiazol-3-ium) tetrakis(2-nitrobenzoate) VAYYIE	$R_2^2(8)$, $R_4^2(8)$, $S(6)$ Intramolecular interaction between (Nitro)O....O (carboxylate)	(Nitro)O...S(thiazole), 3D	Liu,B.-X.; Yu,J.-Y.;Xu,D.-J.*Acta Crystallogr., Sect.E: Struct.Rep. Online* **2005**,61, o4119
v	2,2'-Diamino-4,4'-bi-1,3-thiazolium bis(3-nitrobenzoate) EHACIA	$R_2^2(8), R_4^2(8)$	(Nitro)O...S(thiazole), 3D	Liu,B.-X.;Yu,Y.-P.; Lin,Y.;Du, M. *Acta Crystallogr. Sect.E: Struct.Rep. Online* **2009**,65, o590

vi	bis(2-Aminothiazolium) succinate succinic acid MOSMIR	$R_2^2(8)$	(COOH)O-H...O$^-$(COO$^-$), (thiazole)S...O(COOH), 3D	Fun, H.-K.; John,J.; Jebas,S.R.; Balasubramanian, T. *Acta Crystallogr., Sect. E:Struct.Rep.Online* **2009**,65, o744
vii	2-amino-1,3-thiazolium hydrogen maleate DUZPUK	$R_2^2(8), S(7)$	(thiazole)S...O(COOH), 3D	John,J.; Balasubramanian,T. *Acta Crystallogr., Sect.C:Cryst.Struct.Commun.***2010**,66,o436
viii	2-amino-1,3-thiazolium hydrogen fumarate DUZQAR	$R_2^2(8)$	(COOH)O-H...O$^-$ (COO$^-$), 3D	John,J.; Balasubramanian,T. *Acta Crystallogr., Sect.C: Cryst. Struct.Commun.* **2010**, 66,o436
ix	2-Amino-4-phenylthiazolium hemikis(phthalate) ISIBUI	$R_2^2(8)$	(amine)N-H...O, (thiazole)S...O(COO$^-$), 3D	Jin,S.; Zhang,W.; Liu,L.; Wang,D.; He,H.; Shi,T.; Lin,F. *J. Mol. Struct.* **2011**, 991,1
x	2-Amino-4-phenylthiazolium hydrogen maleate ISICIX	$R_2^2(8), S(7)$	(thiazole)S...O(COOH), 2D	Jin,S.; Zhang,W.; Liu,L.; Wang,D.; He,H.;Shi,T.;Lin,F. *J. Mol. Struct.* **2011**, 991,1

xi	(-)-2,6-Diamino-4,5,6,7-tetrahydrobenzothiazole (L)-(+)-tartrate trihydrate FECZES	R_2^2 (8)	(thiazole)S...O(COO^-), (hydroxyl)O-H...O(water), 3D	Schneider, C.S.; Mierau,J. *J.Med.Chem* .**1987,** 30, 494
xii	2-Aminothiazolium trichloroacetate CUDREY	R_2^2 (8)	Cl...π(thiazole), (thiazole)S...C(COO^-)	Kuz'mina,L. G.; Struchkov, Y.T. *J. Struc. Chem.* **1984**, 25, 917
xiii	2-Amino-5-methyl-1,3-thiazolium-4-nitrobenzoate XUVPOU	R_2^2 (8)	(thiazole)S...O(Nitro)	Lynch, D.E. *Private Communication* **2009**.
xiv	2-Amino-5-methyl-1,3-thiazolium 2-amino-5-methyl-1,3-thiazole 2-(2-(2,6-dichlorophenylamino) phenyl)acetic acid 2-(2-(2,6-dichlorophenylamino) phenyl)acetate XUVQEL	R_2^2 (8)	(thiazole)S...N(amine), (amine)N-H....O^-(COO^-)	Lynch, D.E. *Private Communication* **2009**.

Table S1: b) List of compounds obtained after CSD search of 2-aminothiazoline based organic salts/ cocrystals

S. No.	Name of the Compounds CSD REFCODE	Supramolecular Synthon (graph set representation)	Weak secondary non-covalent interactions and overall Supramolecular assembly	References
i	2-Amino-2-thiazolinium 2-naphthoxyacetate IZEDAS	R_2^2 (8)	C-H…S(thiazoline), C-H…O, 3D	Lynch, D.E. *Acta Crystallogr.,Sect.C: Cryst.Struct.Commun.* **2004** ,60**,** o677
ii	2-Amino-2-thiazolinium indole-2-carboxylate QAGJAJ	R_2^2 (8)	(thiazoline)S… π , 3D	Lynch, D.E., Nicholls, L.J., Smith, G., Byriel, K.A., Kennard, C.H.L. *Acta*

				*Crystallogr.,Sect.B: Struct. Sci.,***1999** *,* 55, 758
iii	2-Amino-2-thiazolinium N-methylpyrrole-2-carboxylate QAGJEN	R_2^2 (8)	(thiazoline)S… π , C-H…O, 3D	Lynch, D.E., Nicholls, L.J., Smith, G., Byriel, K.A., Kennard, C.H.L. *Acta Crystallogr.,Sect.B: Struct. Sci.,***1999** *,* 55, 758
iv	2-Amino-2-thiazolium (2,5-dichlorophenoxy)acetate RADDUW	R_2^2 (8)	N-H…O, Cl…Cl, Cl…S (thiazoline), 3D	Lynch, D.E., Barfield, J., Frost, J., Antrobus, R., Simmons, J. *Crystal Engineering*, **2003** *,*6,109
v	2-Amino-2-thiazolium (2,6-dichlorophenoxy)acetate (2,6-dichlorophenoxy)acetic acid RADFIM	R_2^2 (8)	(thiazoline)S…N (thiazoline), Cl… π , 3D	Lynch, D.E., Barfield, J., Frost, J., Antrobus, R., Simmons, J. *Crystal Engineering*, **2003** *,*6, 109
vi	2-Amino-2-thiazolinium (2,3-dichlorophenoxy)acetate RADFUY	R_2^2 (8)	C-H…S(thiazoline), C-H…Cl, 3D	Lynch, D.E., Barfield, J., Frost, J., Antrobus, R., Simmons, J. *Crystal Engineering*, **2003** *,*6, 109
vii	2-Aminothiazolinium 2-aminobenzoate VAPLIH	R_2^2 (8)	(thiazoline)S…O, C-H…O, 3D	Lynch, D.E., Smith, G. Byriel, K.A., Kennard C.H.L. *Aust. J.Chem.* **1998** *,*51, 587

viii	2-Amino-2-thiazoline (2,4,5-trichlorophenoxy)acetic acid XAPXAN	R_2^2 (8)	(thiazoline)S…Cl, Cl…Cl, C-H…O, 3D	Lynch, D.E., Cooper, C.J., Chauhan, V., Smith, Healy, G. P., Parsons, S. *Aust.J.Chem.* **1999** ,52, 695

Table-S2: Gelation Behaviour of B1A1-B3A7

Solvent	B1A1	B1A2	B1A3	B1A4	B1A5	B1A6	B1A6a	B1A7	B2A1	B2A2	B2A3	B2A4
Water	S	S	S	S	S	S	S	S	S	S	S	S
Methanol	S	S	S	S	S	S	S	S	S	S	S	S
Ethanol	S	S	S	S	S	S	S	S	S	S	S	S
1-pentanol	C	C	S	S	P	P	P	P	S	S	S	S
1-Heptanol	S	S	S	S	S	S	S	S	S	S	S	S
Iso-octane	S	S	P	P	P	P	P	P	S	S	P	P
n-octadecane	S	S	S	S	S	S	S	S	S	S	S	S
Toluene	P	P	S	S	S	S	S	S	P	P	S	S
Xylene	C	C	C	C	C	S	S	S	C	C	C	S

Solvent	B2A5	B2A6	B2A6a	B2A7	B3A1	B3A2	B3A3	B3A4	B3A5	B3A6	B3A6a	B3A7
Water	S	S	S	S	S	S	S	S	S	**G (4.34)**	S	S
Methanol	S	S	S	S	S	S	S	S	S	S	S	S
Ethanol	S	S	S	S	S	S	S	S	S	S	S	S
1-pentanol	P	P	P	P	S	S	S	S	P	P	P	P
1-Heptanol	S	S	S	S	S	S	S	S	S	S	S	S
Iso-octane	P	P	P	P	S	S	P	P	P	P	P	P
n-octadecane	S	S	S	S	S	S	S	S	S	S	S	S
Toluene	S	S	S	P	P	P	P	P	P	P	P	P
Xylene	C	S	S	C	C	C	C	C	C	S	S	S

C=crystal, p=ppt , G=gel, s=solution, the values within the bracket represents MGC (in wt %)

Table S3: Crystallographic information of salt/ cocrystals

	B1A3	**B1A4**	**B1A5**	**B1A6**	**B2A5**	**B2A6**
Empirical Formula	$C_6\ H_8\ N_2O_4S_1$	$C_9H_{16}N_2O_5S_1$	$C_7H_{11}N_2O_2S_1$	$C_{16}H_{26}N_4O_4S_2$	$C_{16}\ H_{26}\ N_4\ O_4\ S_2$	$C_{18}H_{30}N_4O_4S_2$
Fw	204.21	264.30	187.24	402.55	402.54	430.60
Crystal size (mm^3)	0.27×0.21× 0.18	0.60×0.59× 0.15	0.85×0.65× 0.18	0.48×0.13× 0.12	0.32×0.27× 0.18	0.42×0.21× 0.20
Crystal system	monoclinic	Triclinic	Monoclinic	Monoclinic	monoclinic	Monoclinic
Space group	P 2_1	P-1	$P2_1/n$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a/A^0	6.3856(5)	4.95459(19)	9.0290(3)	8.4023(6)	5.2800(2)	8.702(6)
b/A^0	6.6445(5)	7.5581(3)	5.75526(18)	7.5547(5)	22.5958(11)	7.721(5)
c/A^0	10.5589(8)	17.8016(6)	18.2666(6)	17.3163(12)	8.6882(4)	17.891(13)
α/deg	90	92.253(3)	90.00	90.00	90.00	90.00
β/deg	91.304(7)	90.649(3)	98.566(3)	103.335(2)	97.882(4)	95.326(14)
γ/deg	90	109.029(4)	90.00	90.00	90.00	90.00
Volume $(A^0)^{-3}$	447.76(6)	629.50(4)	938.62(6)	1069.55(13)	1026.76(8)	1196.9(14)
Z	2	1	2	2	2	2
$D_{calc.}$	1.514	1.394	1.325	1.250	1.302	1.195
F(000)	212	280	396	428	428	460
μ(MoKα) (mm^{-1})	3.161	2.432	2.796	0.275	2.591	0.250
Temperature(K)	293(2)	298	298(2)	298(2)	293	293(2)
obsd reflns [$I > 2\sigma(I)$]	1477	2290	1763	1872	1452	2090
params refined	126	188	120	127	131	138
goodness of fit	1.645	0.991	1.201	1.136	0.840	0.902
final R1 on obsd data	0.0645	0.0526	0.0494	0.0478	0.0546	0.0424
final wR2 on obsd data	0.2109	0.1553	0.1547	0.1174	0.1828	0.1167
CCDC No.	989348	964477	964476	930266	989346	949111

	B3A1	**B3A2**	**B3A6**	**B3A7**	**B3A6a**
Empirical formula	$C_{32}H_{40}N_8O_{16}S_4$	$C_8H_{10}N_2O_4S_1$	$C_{14}H_{24}N_2O_4S_1$	$C_{20}H_{34}N_4O_4S_2$	C_{36} H_{60} N_8 O_8 S_4
Fw	920.98	230.25	316.42	458.65	861.19
Crystal size (mm^3)	0.98×0.60 ×0.15	0.42×0.21× 0.20	0.42×0.21× 0.21	0.90×0.58× 0.16	0.29×0.25× 0.18
Crystal system	Monoclinic	Monoclinic	Monoclinic	Triclinic	monoclinic
Space group	$P2_1/n$	C 2/c	$P2_1/n$	P-1	$P2_1/n$
a/A^0	4.16465(11)	20.921(6)	12.800(17)	7.8169(4)	11.3596(3)
b/A^0	22.5580(7)	9.511(3)	4.945(7)	7.8365(6)	14.6265(7)
c/A^0	10.8698(3)	10.886(3)	27.64(4)	11.4009(8)	13.1548(4)
α/deg	90.00	90.00	90.00	73.310(6)	90.00
β/deg	93.487(2)	103.274(4)	94.730(19)	82.018(5)	91.993(3)
γ/deg	90.00	90.00	90.00	65.685(6)	90.00
Volume $(A^0)^{-3}$	1019.29(5)	2108.2(11)	1744(4)	609.17(7)	2184.36(14)
Z	4	4	4	1	4
$D_{calc.}$	1.500	1.464	1.205	1.250	1.309
F(000)	480	976	680	246	920
μ(MoKα) (mm^{-1})	2.848	0.301	0.201	2.243	2.470
Temperature(K)	298	298(2)	298(2)	298	293
obsd reflns [$I > 2\sigma(I)$]	3429	3590	2443	2326	4188
params refined	176	142	193	145	271
goodness of fit	1.493	1.284	0.986	0.761	1.622
final R1 on obsd data	0.0473	0.0540	0.0756	0.0459	0.0722
final wR2 on obsd data	0.1684	0.1581	0.1981	0.1558	0.2265
CCDC No.	958280	949112	930265	958299	989347