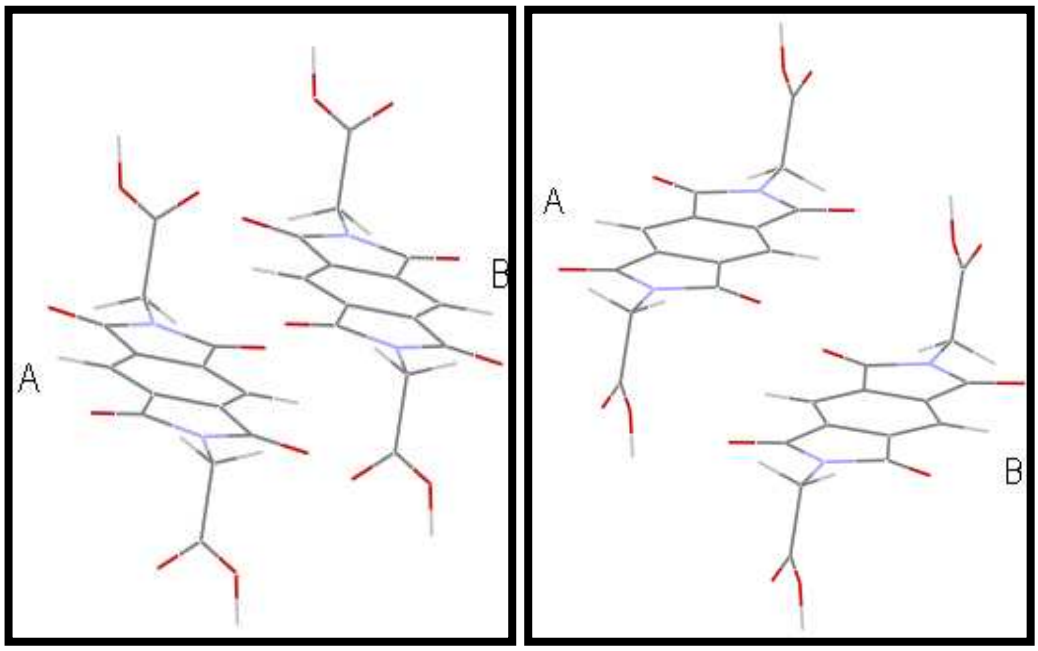
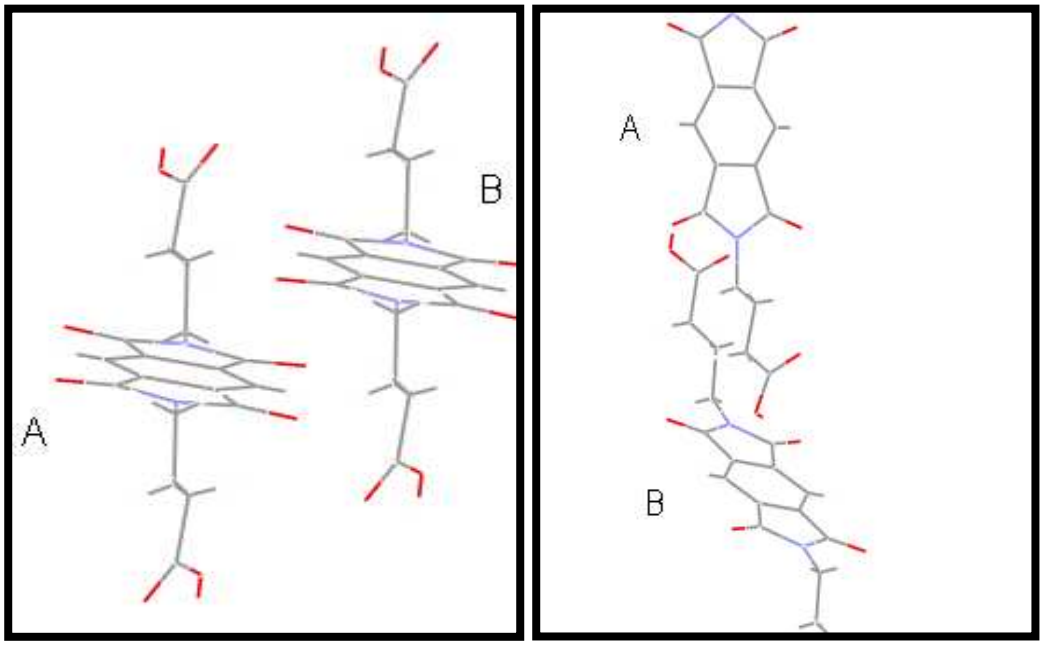
Appendix: A1 – Lattice Energy Tables



(a) (b)

Figure A1.1: 3D offset arrangement of gly-L molecules corresponding to (a) -61.4kJ/mol and (b) -44.4kJ/mol.



(a) (b)

Figure A1.2: (a) 3D offset arrangement of but-L molecules corresponding to -63.8kJ/mol (b) 2D offset arrangement corresponding to -32.5kJ/mol.

Table A1.1: Tabulated molecule-molecule interaction energies for gly-L.

1:	1	1	-1.00+x,	y,	z	-61.4	kJ/mol	5.07 Ang
2:	1	1	1.00+x,	y,	z	-61.4	kJ/mol	5.07 Ang
3:	1	1	x,	-1.00+y,	-1.00+z	-49.7	kJ/mol	13.55 Ang
4:	1	1	x,	1.00+y,	1.00+z	-49.7	kJ/mol	13.55 Ang
5:	1	1	x,	-1.00+y,	z	-44.4	kJ/mol	5.19 Ang
6:	1	1	x,	1.00+y,	z	-44.4	kJ/mol	5.19 Ang
7:	1	1	x,	y,	-1.00+z	-20.1	kJ/mol	12.43 Ang
8:	1	1	x,	y,	1.00+z	-20.1	kJ/mol	12.43 Ang
9:	1	1	-1.00+x,	-1.00+y,	z	-11.6	kJ/mol	7.71 Ang
10:	1	1	1.00+x,	1.00+y,	z	-11.6	kJ/mol	7.71 Ang
11:	1	1	-1.00+x,	y,	-1.00+z	-11.3	kJ/mol	13.97 Ang
12:	1	1	1.00+x,	y,	1.00+z	-11.3	kJ/mol	13.97 Ang
13:	1	1	-1.00+x,	1.00+y,	z	-9.1	kJ/mol	6.77 Ang
14:	1	1	1.00+x,	-1.00+y,	z	-9.1	kJ/mol	6.77 Ang
15:	1	1	-1.00+x,	-1.00+y,	-1.00+z	-7.1	kJ/mol	15.20 Ang
16:	1	1	1.00+x,	1.00+y,	1.00+z	-7.1	kJ/mol	15.20 Ang
17:	1	1	-2.00+x,	y,	z	-1.6	kJ/mol	10.13 Ang
18:	1	1	2.00+x,	y,	z	-1.6	kJ/mol	10.13 Ang
19:	1	1	-1.00+x,	y,	1.00+z	-1.4	kJ/mol	12.84 Ang
20:	1	1	x,	-1.00+y,	1.00+z	-1.4	kJ/mol	13.39 Ang
21:	1	1	x,	1.00+y,	-1.00+z	-1.4	kJ/mol	13.39 Ang
22:	1	1	1.00+x,	y,	-1.00+z	-1.4	kJ/mol	12.84 Ang
23:	1	1	x,	-2.00+y,	z	-1.2	kJ/mol	10.38 Ang
24:	1	1	x,	2.00+y,	z	-1.2	kJ/mol	10.38 Ang
25:	1	1	-1.00+x,	1.00+y,	1.00+z	-1.1	kJ/mol	13.68 Ang
26:	1	1	1.00+x,	-1.00+y,	-1.00+z	-1.1	kJ/mol	13.68 Ang
27:	1	1	-1.00+x,	1.00+y,	-1.00+z	-1.0	kJ/mol	14.60 Ang
28:	1	1	1.00+x,	-1.00+y,	1.00+z	-1.0	kJ/mol	14.60 Ang

Sum of above Molecule-Molecule interactions: -444.80 kJ/mol

Table A1.2: Tabulated molecule-molecule interaction energies for gly-NAP.

1:	1	2	x,	y,	z	-53.4	kJ/mol	3.44 Ang
2:	2	1	-1.00+x,	y,	z	-53.4	kJ/mol	3.44 Ang
3:	1	2	1.00+x,	y,	z	-53.4	kJ/mol	3.44 Ang
4:	1	1	x,	-1.00+y,	-1.00+z	-48.0	kJ/mol	13.99 Ang
5:	1	1	x,	1.00+y,	1.00+z	-48.0	kJ/mol	13.99 Ang
6:	1	1	x,	-1.00+y,	z	-26.0	kJ/mol	7.61 Ang
7:	1	1	x,	1.00+y,	z	-26.0	kJ/mol	7.61 Ang
8:	1	1	x,	y,	-1.00+z	-14.4	kJ/mol	10.48 Ang
9:	1	1	x,	y,	1.00+z	-14.4	kJ/mol	10.48 Ang
10:	1	1	-1.00+x,	y,	1.00+z	-13.8	kJ/mol	10.48 Ang
11:	1	1	1.00+x,	y,	-1.00+z	-13.8	kJ/mol	10.48 Ang
12:	1	1	-1.00+x,	1.00+y,	1.00+z	-10.5	kJ/mol	13.60 Ang
13:	1	1	1.00+x,	-1.00+y,	-1.00+z	-10.5	kJ/mol	13.60 Ang
14:	2	1	-1.00+x,	y,	1.00+z	-9.6	kJ/mol	9.90 Ang
15:	2	1	x,	y,	-1.00+z	-9.6	kJ/mol	9.90 Ang
16:	1	2	x,	y,	1.00+z	-9.6	kJ/mol	9.90 Ang
17:	1	2	1.00+x,	y,	-1.00+z	-9.6	kJ/mol	9.90 Ang
18:	2	1	-1.00+x,	1.00+y,	z	-8.0	kJ/mol	8.01 Ang
19:	2	1	x,	-1.00+y,	z	-8.0	kJ/mol	8.01 Ang
20:	1	2	x,	1.00+y,	z	-8.0	kJ/mol	8.01 Ang
21:	1	2	1.00+x,	-1.00+y,	z	-8.0	kJ/mol	8.01 Ang

```
22:   1  1 -1.00+x,       y,       z    -7.9 kJ/mol   6.88 Ang
23:   1  1  1.00+x,       y,       z    -7.9 kJ/mol   6.88 Ang
24:   2  2       x, -1.00+y,       z    -4.6 kJ/mol   7.61 Ang
25:   2  2       x,  1.00+y,       z    -4.6 kJ/mol   7.61 Ang
26:   2  1 -1.00+x, -1.00+y,       z    -3.3 kJ/mol   8.67 Ang
27:   1  2       x, -1.00+y,       z    -3.3 kJ/mol   8.67 Ang
28:   2  1       x,  1.00+y,       z    -3.3 kJ/mol   8.67 Ang
29:   1  2  1.00+x,  1.00+y,       z    -3.3 kJ/mol   8.67 Ang
30:   2  1 -1.00+x,  1.00+y,  1.00+z    -3.0 kJ/mol  13.36 Ang
31:   2  1       x, -1.00+y, -1.00+z    -3.0 kJ/mol  13.36 Ang
32:   1  2       x,  1.00+y,  1.00+z    -3.0 kJ/mol  13.36 Ang
33:   1  2  1.00+x, -1.00+y, -1.00+z    -3.0 kJ/mol  13.36 Ang
34:   1  1 -1.00+x,  1.00+y,       z    -2.4 kJ/mol   9.71 Ang
35:   1  1  1.00+x, -1.00+y,       z    -2.4 kJ/mol   9.71 Ang
36:   2  2 -1.00+x,       y,       z    -2.0 kJ/mol   6.88 Ang
37:   2  2  1.00+x,       y,       z    -2.0 kJ/mol   6.88 Ang
38:   1  1 -1.00+x, -1.00+y,       z    -1.2 kJ/mol  10.78 Ang
39:   1  1  1.00+x,  1.00+y,       z    -1.2 kJ/mol  10.78 Ang

Sum of above Molecule-Molecule interactions: -517.40 kJ/mol
```

Table A1.3: Tabulated molecule-molecule interaction energies for gly-ANT.

```
1:    1  4       x,       y,       z   -65.8 kJ/mol   3.92 Ang
2:    1  4 -1.00+x,       y,       z   -65.8 kJ/mol   3.92 Ang
3:    4  1  1.00+x,       y,       z   -65.8 kJ/mol   3.92 Ang
4:    1  2       x,       y,       z   -25.6 kJ/mol   7.51 Ang
5:    1  3       x,       y,       z   -25.6 kJ/mol   7.52 Ang
6:    1  2       x, -1.00+y,       z   -21.0 kJ/mol   9.57 Ang
7:    3  1       x, -1.00+y,       z   -21.0 kJ/mol   9.56 Ang
8:    1  3       x,  1.00+y,       z   -21.0 kJ/mol   9.56 Ang
9:    2  1       x,  1.00+y,       z   -21.0 kJ/mol   9.57 Ang
10:   1  1      -x,  0.50+y,  0.50-z   -17.8 kJ/mol   9.78 Ang
11:   1  1      -x, -0.50+y,  0.50-z   -17.8 kJ/mol   9.78 Ang
12:   1  1      -x, -0.50+y,  1.50-z   -17.8 kJ/mol   9.78 Ang
13:   1  1      -x,  0.50+y,  1.50-z   -17.8 kJ/mol   9.78 Ang
14:   1  4      -x,  0.50+y,  0.50-z   -10.0 kJ/mol   9.99 Ang
15:   4  1      -x, -0.50+y,  0.50-z   -10.0 kJ/mol   9.99 Ang
16:   1  4  1.00-x, -0.50+y,  1.50-z   -10.0 kJ/mol   9.99 Ang
17:   4  1  1.00-x,  0.50+y,  1.50-z   -10.0 kJ/mol   9.99 Ang
18:   4  1      -x,  0.50+y,  0.50-z    -9.4 kJ/mol   9.99 Ang
19:   1  4      -x, -0.50+y,  0.50-z    -9.4 kJ/mol   9.99 Ang
20:   4  1  1.00-x, -0.50+y,  1.50-z    -9.4 kJ/mol   9.99 Ang
21:   1  4  1.00-x,  0.50+y,  1.50-z    -9.4 kJ/mol   9.99 Ang
22:   2  1      -x,  0.50+y,  0.50-z    -8.0 kJ/mol   4.95 Ang
23:   1  2      -x, -0.50+y,  0.50-z    -8.0 kJ/mol   4.95 Ang
24:   3  1      -x, -0.50+y,  1.50-z    -7.9 kJ/mol   4.95 Ang
25:   1  3      -x,  0.50+y,  1.50-z    -7.9 kJ/mol   4.95 Ang
26:   4  3      -x,  0.50+y,  0.50-z    -6.1 kJ/mol   5.26 Ang
27:   3  4      -x, -0.50+y,  0.50-z    -6.1 kJ/mol   5.26 Ang
28:   4  2  1.00-x, -0.50+y,  1.50-z    -6.1 kJ/mol   5.26 Ang
29:   2  4  1.00-x,  0.50+y,  1.50-z    -6.1 kJ/mol   5.26 Ang
30:   1  2 -1.00+x,       y,       z    -4.9 kJ/mol   9.32 Ang
31:   3  1 -1.00+x,       y,       z    -4.9 kJ/mol   9.32 Ang
32:   1  3  1.00+x,       y,       z    -4.9 kJ/mol   9.32 Ang
```

```
33:   2  1  1.00+x,       y,       z    -4.9 kJ/mol   9.32 Ang
34:   1  1 -1.00+x,       y,       z    -4.6 kJ/mol   7.84 Ang
35:   1  1  1.00+x,       y,       z    -4.6 kJ/mol   7.84 Ang
36:   4  4  1.00-x, -0.50+y,  0.50-z    -4.2 kJ/mol   9.78 Ang
37:   4  4  1.00-x, -0.50+y,  1.50-z    -4.2 kJ/mol   9.78 Ang
38:   4  4  1.00-x,  0.50+y,  0.50-z    -4.2 kJ/mol   9.78 Ang
39:   4  4  1.00-x,  0.50+y,  1.50-z    -4.2 kJ/mol   9.78 Ang
40:   3  2       x, -1.00+y,       z    -3.9 kJ/mol   4.51 Ang
41:   2  3       x,  1.00+y,       z    -3.9 kJ/mol   4.51 Ang
42:   3  4      -x, -0.50+y,  1.50-z    -3.7 kJ/mol   5.96 Ang
43:   4  3      -x,  0.50+y,  1.50-z    -3.7 kJ/mol   5.96 Ang
44:   4  2  1.00-x, -0.50+y,  0.50-z    -3.7 kJ/mol   5.96 Ang
45:   2  4  1.00-x,  0.50+y,  0.50-z    -3.7 kJ/mol   5.96 Ang
46:   3  4 -1.00+x,       y,       z    -3.6 kJ/mol   7.50 Ang
47:   4  3  1.00+x,       y,       z    -3.6 kJ/mol   7.50 Ang
48:   3  1 -1.00-x, -0.50+y,  0.50-z    -3.3 kJ/mol   6.86 Ang
49:   1  3 -1.00-x,  0.50+y,  0.50-z    -3.3 kJ/mol   6.86 Ang
50:   1  2  1.00-x, -0.50+y,  1.50-z    -3.3 kJ/mol   6.86 Ang
51:   2  1  1.00-x,  0.50+y,  1.50-z    -3.3 kJ/mol   6.86 Ang
52:   2  4       x,       y,       z    -3.1 kJ/mol   7.50 Ang
53:   1  1 -1.00-x, -0.50+y,  0.50-z    -2.5 kJ/mol  11.61 Ang
54:   1  1 -1.00-x,  0.50+y,  0.50-z    -2.5 kJ/mol  11.61 Ang
55:   1  1  1.00-x, -0.50+y,  1.50-z    -2.5 kJ/mol  11.61 Ang
56:   1  1  1.00-x,  0.50+y,  1.50-z    -2.5 kJ/mol  11.61 Ang
57:   1  3      -x,  0.50+y,  0.50-z    -2.4 kJ/mol   6.25 Ang
58:   4  4 -1.00+x,       y,       z    -2.4 kJ/mol   7.84 Ang
59:   3  1      -x, -0.50+y,  0.50-z    -2.4 kJ/mol   6.25 Ang
60:   1  2      -x, -0.50+y,  1.50-z    -2.4 kJ/mol   6.25 Ang
61:   4  1      -x, -0.50+y,  1.50-z    -2.4 kJ/mol  11.05 Ang
62:   1  4      -x,  0.50+y,  1.50-z    -2.4 kJ/mol  11.05 Ang
63:   2  1      -x,  0.50+y,  1.50-z    -2.4 kJ/mol   6.25 Ang
64:   1  4  1.00-x, -0.50+y,  0.50-z    -2.4 kJ/mol  11.05 Ang
65:   4  4  1.00+x,       y,       z    -2.4 kJ/mol   7.84 Ang
66:   4  1  1.00-x,  0.50+y,  0.50-z    -2.4 kJ/mol  11.05 Ang
67:   1  1       x, -1.00+y,       z    -1.7 kJ/mol  16.60 Ang
68:   1  1       x,  1.00+y,       z    -1.7 kJ/mol  16.60 Ang
69:   1  4      -x, -0.50+y,  1.50-z    -1.6 kJ/mol  11.05 Ang
70:   4  1      -x,  0.50+y,  1.50-z    -1.6 kJ/mol  11.05 Ang
71:   4  1  1.00-x, -0.50+y,  0.50-z    -1.6 kJ/mol  11.05 Ang
72:   1  4  1.00-x,  0.50+y,  0.50-z    -1.6 kJ/mol  11.05 Ang
73:   2  4      -x,  0.50+y,  0.50-z    -1.4 kJ/mol   6.65 Ang
74:   4  2      -x, -0.50+y,  0.50-z    -1.4 kJ/mol   6.65 Ang
75:   3  4  1.00-x, -0.50+y,  1.50-z    -1.4 kJ/mol   6.66 Ang
76:   4  3  1.00-x,  0.50+y,  1.50-z    -1.4 kJ/mol   6.66 Ang
77:   1  4 -1.00+x,       y, -1.00+z    -1.3 kJ/mol   9.99 Ang
78:   1  1       x,       y, -1.00+z    -1.3 kJ/mol  10.33 Ang
79:   4  1       x,       y, -1.00+z    -1.3 kJ/mol   9.99 Ang
80:   1  1       x,       y,  1.00+z    -1.3 kJ/mol  10.33 Ang
81:   1  4       x,       y,  1.00+z    -1.3 kJ/mol   9.99 Ang
82:   4  1  1.00+x,       y,  1.00+z    -1.3 kJ/mol   9.99 Ang
83:   3  2 -1.00+x, -1.00+y,       z    -1.2 kJ/mol   4.42 Ang
84:   2  3  1.00+x,  1.00+y,       z    -1.2 kJ/mol   4.42 Ang

Sum of above Molecule-Molecule interactions: -688.90 kJ/mol
```

Table A1.4: Tabulated molecule-molecule interaction energies for gly-PHEN.

1:	1	2	x,	y,	z	-65.2 kJ/mol	3.85 Ang
2:	2	1	x,	-1.00+y,	z	-61.7 kJ/mol	4.03 Ang
3:	1	2	x,	1.00+y,	z	-61.7 kJ/mol	4.03 Ang
4:	1	1	2.00-x,	2.00-y,	-z	-49.3 kJ/mol	12.74 Ang
5:	1	1	-x,	2.00-y,	1.00-z	-42.4 kJ/mol	14.39 Ang
6:	1	1	-1.00+x,	y,	z	-31.7 kJ/mol	7.49 Ang
7:	1	1	1.00+x,	y,	z	-31.7 kJ/mol	7.49 Ang
8:	1	1	1.00-x,	2.00-y,	1.00-z	-14.0 kJ/mol	10.60 Ang
9:	1	2	-1.00+x,	1.00+y,	z	-13.7 kJ/mol	8.96 Ang
10:	2	1	1.00+x,	-1.00+y,	z	-13.7 kJ/mol	8.96 Ang
11:	1	2	1.00-x,	1.00-y,	-z	-11.9 kJ/mol	10.29 Ang
12:	2	1	1.00-x,	1.00-y,	-z	-11.9 kJ/mol	10.29 Ang
13:	1	1	1.00-x,	1.00-y,	-z	-11.6 kJ/mol	10.88 Ang
14:	1	1	2.00-x,	1.00-y,	-z	-10.3 kJ/mol	14.01 Ang
15:	2	2	-1.00+x,	y,	z	-10.0 kJ/mol	7.49 Ang
16:	2	2	1.00+x,	y,	z	-10.0 kJ/mol	7.49 Ang
17:	2	1	-1.00+x,	y,	z	-9.1 kJ/mol	8.58 Ang
18:	1	2	1.00+x,	y,	z	-9.1 kJ/mol	8.58 Ang
19:	1	2	1.00-x,	2.00-y,	1.00-z	-8.6 kJ/mol	10.93 Ang
20:	2	1	1.00-x,	2.00-y,	1.00-z	-8.6 kJ/mol	10.93 Ang
21:	2	2	1.00-x,	1.00-y,	1.00-z	-7.8 kJ/mol	9.17 Ang
22:	1	1	1.00-x,	2.00-y,	-z	-6.9 kJ/mol	9.75 Ang
23:	1	1	x,	-1.00+y,	z	-5.1 kJ/mol	7.75 Ang
24:	1	1	x,	1.00+y,	z	-5.1 kJ/mol	7.75 Ang
25:	1	2	-1.00+x,	y,	z	-4.9 kJ/mol	8.26 Ang
26:	2	1	1.00+x,	y,	z	-4.9 kJ/mol	8.26 Ang
27:	2	1	-1.00+x,	-1.00+y,	z	-4.8 kJ/mol	8.03 Ang
28:	1	2	1.00+x,	1.00+y,	z	-4.8 kJ/mol	8.03 Ang
29:	1	2	2.00-x,	1.00-y,	-z	-3.6 kJ/mol	13.45 Ang
30:	2	1	2.00-x,	1.00-y,	-z	-3.6 kJ/mol	13.45 Ang
31:	1	2	1.00-x,	1.00-y,	1.00-z	-2.8 kJ/mol	10.29 Ang
32:	2	1	1.00-x,	1.00-y,	1.00-z	-2.8 kJ/mol	10.29 Ang
33:	2	2	x,	-1.00+y,	z	-2.5 kJ/mol	7.75 Ang
34:	2	2	x,	1.00+y,	z	-2.5 kJ/mol	7.75 Ang
35:	1	2	-x,	2.00-y,	1.00-z	-2.0 kJ/mol	14.73 Ang
36:	2	1	-x,	2.00-y,	1.00-z	-2.0 kJ/mol	14.73 Ang
37:	1	1	-1.00+x,	1.00+y,	z	-1.9 kJ/mol	11.26 Ang
38:	1	1	1.00+x,	-1.00+y,	z	-1.9 kJ/mol	11.26 Ang
39:	1	1	1.00-x,	3.00-y,	1.00-z	-1.7 kJ/mol	13.69 Ang
40:	2	2	2.00-x,	1.00-y,	1.00-z	-1.3 kJ/mol	10.33 Ang
41:	2	2	1.00-x,	-y,	-z	-1.2 kJ/mol	12.21 Ang
42:	1	1	-1.00+x,	-1.00+y,	z	-1.1 kJ/mol	10.28 Ang
43:	1	1	1.00+x,	1.00+y,	z	-1.1 kJ/mol	10.28 Ang
44:	1	1	2.00-x,	2.00-y,	1.00-z	-1.1 kJ/mol	11.39 Ang

Sum of above Molecule-Molecule interactions: -563.60 kJ/mol

Table A1.5: Tabulated molecule-molecule interaction energies for gly-PERY.

1:	1	2	x,	y,	z	-72.0 kJ/mol	4.41 Ang
2:	2	1	x,	-1.00+y,	z	-72.0 kJ/mol	4.41 Ang
3:	1	2	x,	1.00+y,	z	-72.0 kJ/mol	4.41 Ang
4:	1	1	-1.00+x,	y,	-1.00+z	-47.5 kJ/mol	14.28 Ang
5:	1	1	1.00+x,	y,	1.00+z	-47.5 kJ/mol	14.28 Ang

```
6:    1  1 -1.00+x,       y,       z   -32.3 kJ/mol   7.24 Ang
7:    1  1  1.00+x,       y,       z   -32.3 kJ/mol   7.24 Ang
8:    2  2 -1.00+x,       y,       z   -23.2 kJ/mol   7.24 Ang
9:    2  2  1.00+x,       y,       z   -23.2 kJ/mol   7.24 Ang
10:   2  1 -1.00+x, -1.00+y,       z   -14.7 kJ/mol   9.24 Ang
11:   1  2 -1.00+x,       y,       z   -14.7 kJ/mol   9.24 Ang
12:   2  1  1.00+x,       y,       z   -14.7 kJ/mol   9.24 Ang
13:   1  2  1.00+x,  1.00+y,       z   -14.7 kJ/mol   9.24 Ang
14:   1  1       x,       y, -1.00+z   -14.2 kJ/mol  10.80 Ang
15:   1  1       x,       y,  1.00+z   -14.2 kJ/mol  10.80 Ang
16:   2  1       x, -1.00+y, -1.00+z    -9.2 kJ/mol  12.34 Ang
17:   1  2       x,       y, -1.00+z    -9.2 kJ/mol  12.34 Ang
18:   2  1       x,       y,  1.00+z    -9.2 kJ/mol  12.34 Ang
19:   1  2       x,  1.00+y,  1.00+z    -9.2 kJ/mol  12.34 Ang
20:   2  2       x,       y, -1.00+z    -7.1 kJ/mol  10.80 Ang
21:   2  2       x,       y,  1.00+z    -7.1 kJ/mol  10.80 Ang
22:   2  1 -1.00+x,       y,       z    -7.0 kJ/mol   7.63 Ang
23:   1  2 -1.00+x,  1.00+y,       z    -7.0 kJ/mol   7.63 Ang
24:   2  1  1.00+x, -1.00+y,       z    -7.0 kJ/mol   7.63 Ang
25:   1  2  1.00+x,       y,       z    -7.0 kJ/mol   7.63 Ang
26:   1  1       x, -1.00+y,       z    -3.3 kJ/mol   8.82 Ang
27:   1  1       x,  1.00+y,       z    -3.3 kJ/mol   8.82 Ang
28:   2  1       x, -1.00+y,  1.00+z    -3.2 kJ/mol  10.96 Ang
29:   2  1       x,       y, -1.00+z    -3.2 kJ/mol  10.96 Ang
30:   1  2       x,       y,  1.00+z    -3.2 kJ/mol  10.96 Ang
31:   1  2       x,  1.00+y, -1.00+z    -3.2 kJ/mol  10.96 Ang
32:   2  2 -1.00+x,       y,  1.00+z    -3.0 kJ/mol  11.60 Ang
33:   2  2  1.00+x,       y, -1.00+z    -3.0 kJ/mol  11.60 Ang
34:   2  2       x, -1.00+y,       z    -2.8 kJ/mol   8.82 Ang
35:   2  2       x,  1.00+y,       z    -2.8 kJ/mol   8.82 Ang
36:   2  1 -1.00+x,       y,  1.00+z    -1.3 kJ/mol  12.51 Ang
37:   1  2 -1.00+x,  1.00+y,  1.00+z    -1.3 kJ/mol  12.51 Ang
38:   2  1  1.00+x, -1.00+y, -1.00+z    -1.3 kJ/mol  12.51 Ang
39:   1  2  1.00+x,       y, -1.00+z    -1.3 kJ/mol  12.51 Ang
40:   1  1 -1.00+x,       y,  1.00+z    -1.1 kJ/mol  11.60 Ang
41:   1  1       x, -1.00+y, -1.00+z    -1.1 kJ/mol  15.06 Ang
42:   1  1       x,  1.00+y,  1.00+z    -1.1 kJ/mol  15.06 Ang
43:   1  1  1.00+x,       y, -1.00+z    -1.1 kJ/mol  11.60 Ang

Sum of above Molecule-Molecule interactions: -628.80 kJ/mol
```

Table A1.6: Tabulated molecule-molecule interaction energies for but-L.

```
1:    1  1 -1.00+x,       y,       z   -63.8 kJ/mol   4.95 Ang
2:    1  1  1.00+x,       y,       z   -63.8 kJ/mol   4.95 Ang
3:    1  1       x, -1.00+y,       z   -41.5 kJ/mol  19.23 Ang
4:    1  1       x,  1.00+y,       z   -41.5 kJ/mol  19.23 Ang
5:    1  1 -0.50-x, -0.50+y,  1.50-z   -32.5 kJ/mol  10.79 Ang
6:    1  1 -0.50-x,  0.50+y,  1.50-z   -32.5 kJ/mol  10.79 Ang
7:    1  1  0.50-x, -0.50+y,  2.50-z   -32.5 kJ/mol  10.79 Ang
8:    1  1  0.50-x,  0.50+y,  2.50-z   -32.5 kJ/mol  10.79 Ang
9:    1  1 -0.50-x, -0.50+y,  2.50-z   -25.9 kJ/mol  10.99 Ang
10:   1  1 -0.50-x,  0.50+y,  2.50-z   -25.9 kJ/mol  10.99 Ang
11:   1  1  0.50-x, -0.50+y,  1.50-z   -25.9 kJ/mol  10.99 Ang
12:   1  1  0.50-x,  0.50+y,  1.50-z   -25.9 kJ/mol  10.99 Ang
```

```
13:   1  1 -1.00+x, -1.00+y,       z    -4.7 kJ/mol  19.86 Ang
14:   1  1  1.00+x,  1.00+y,       z    -4.7 kJ/mol  19.86 Ang
15:   1  1       x,       y, -1.00+z    -3.4 kJ/mol   8.93 Ang
16:   1  1       x,       y,  1.00+z    -3.4 kJ/mol   8.93 Ang
17:   1  1 -1.50-x, -0.50+y,  1.50-z    -2.6 kJ/mol  12.69 Ang
18:   1  1 -1.50-x,  0.50+y,  1.50-z    -2.6 kJ/mol  12.69 Ang
19:   1  1  1.50-x, -0.50+y,  2.50-z    -2.6 kJ/mol  12.69 Ang
20:   1  1  1.50-x,  0.50+y,  2.50-z    -2.6 kJ/mol  12.69 Ang
21:   1  1 -1.50-x, -0.50+y,  2.50-z    -1.7 kJ/mol  13.20 Ang
22:   1  1 -2.00+x,       y,       z    -1.7 kJ/mol   9.90 Ang
23:   1  1 -1.50-x,  0.50+y,  2.50-z    -1.7 kJ/mol  13.20 Ang
24:   1  1 -1.00+x,       y, -1.00+z    -1.7 kJ/mol   9.77 Ang
25:   1  1  1.50-x, -0.50+y,  1.50-z    -1.7 kJ/mol  13.20 Ang
26:   1  1  1.00+x,       y,  1.00+z    -1.7 kJ/mol   9.77 Ang
27:   1  1  1.50-x,  0.50+y,  1.50-z    -1.7 kJ/mol  13.20 Ang
28:   1  1  2.00+x,       y,       z    -1.7 kJ/mol   9.90 Ang
29:   1  1 -1.00+x,       y,  1.00+z    -1.4 kJ/mol  10.64 Ang
30:   1  1  1.00+x,       y, -1.00+z    -1.4 kJ/mol  10.64 Ang

Sum of above Molecule-Molecule interactions: -487.20 kJ/mol
```

Table A1.7: Tabulated molecule-molecule interaction energies for but-PHEN.

```
1:    1  2 -1.00+x,       y,       z   -67.1 kJ/mol   3.55 Ang
2:    2  1  1.00+x,       y,       z   -67.1 kJ/mol   3.55 Ang
3:    1  2       x,       y,       z   -64.1 kJ/mol   3.55 Ang
4:    1  1 -1.00+x, -2.00+y, -1.00+z   -46.3 kJ/mol  18.87 Ang
5:    1  1  1.00+x,  2.00+y,  1.00+z   -46.3 kJ/mol  18.87 Ang
6:    1  1       x, -1.00+y,       z   -30.7 kJ/mol  10.40 Ang
7:    1  1       x,  1.00+y,       z   -30.7 kJ/mol  10.40 Ang
8:    1  1       x, -1.00+y, -1.00+z   -22.5 kJ/mol  10.92 Ang
9:    1  1       x,  1.00+y,  1.00+z   -22.5 kJ/mol  10.92 Ang
10:   1  2 -1.00+x, -1.00+y, -1.00+z   -14.0 kJ/mol  10.67 Ang
11:   2  1  1.00+x,  1.00+y,  1.00+z   -14.0 kJ/mol  10.67 Ang
12:   2  1       x, -1.00+y, -1.00+z   -10.8 kJ/mol  10.85 Ang
13:   1  2       x,  1.00+y,  1.00+z   -10.8 kJ/mol  10.85 Ang
14:   1  1       x, -2.00+y, -1.00+z    -9.9 kJ/mol  18.46 Ang
15:   1  1       x,  2.00+y,  1.00+z    -9.9 kJ/mol  18.46 Ang
16:   2  1       x, -1.00+y,       z    -9.8 kJ/mol  10.95 Ang
17:   1  2       x,  1.00+y,       z    -9.8 kJ/mol  10.95 Ang
18:   1  2 -1.00+x, -1.00+y,       z    -9.3 kJ/mol  10.91 Ang
19:   1  1 -1.00+x,       y,       z    -9.3 kJ/mol   7.10 Ang
20:   1  1  1.00+x,       y,       z    -9.3 kJ/mol   7.10 Ang
21:   2  1  1.00+x,  1.00+y,       z    -9.3 kJ/mol  10.91 Ang
22:   1  2 -1.00+x,  1.00+y,       z    -9.1 kJ/mol  11.07 Ang
23:   2  1  1.00+x, -1.00+y,       z    -9.1 kJ/mol  11.07 Ang
24:   1  2       x, -1.00+y,       z    -8.8 kJ/mol  11.03 Ang
25:   2  1       x,  1.00+y,       z    -8.8 kJ/mol  11.03 Ang
26:   1  1 -1.00+x, -1.00+y, -1.00+z    -6.5 kJ/mol  11.73 Ang
27:   1  1  1.00+x,  1.00+y,  1.00+z    -6.5 kJ/mol  11.73 Ang
28:   2  2       x, -1.00+y,       z    -5.0 kJ/mol  10.40 Ang
29:   2  2       x,  1.00+y,       z    -5.0 kJ/mol  10.40 Ang
30:   2  2 -1.00+x,       y,       z    -3.0 kJ/mol   7.10 Ang
31:   2  2  1.00+x,       y,       z    -3.0 kJ/mol   7.10 Ang
32:   1  1 -1.00+x, -1.00+y,       z    -2.0 kJ/mol  12.49 Ang
```

```
33:   1  1  1.00+x,  1.00+y,       z    -2.0 kJ/mol  12.49 Ang
34:   1  1 -1.00+x,  1.00+y,       z    -1.9 kJ/mol  12.70 Ang
35:   1  1  1.00+x, -1.00+y,       z    -1.9 kJ/mol  12.70 Ang
36:   1  2       x, -1.00+y, -1.00+z    -1.7 kJ/mol  12.09 Ang
37:   2  1       x,  1.00+y,  1.00+z    -1.7 kJ/mol  12.09 Ang
38:   1  2 -1.00+x,  1.00+y,  1.00+z    -1.6 kJ/mol  12.24 Ang
39:   2  1  1.00+x, -1.00+y, -1.00+z    -1.6 kJ/mol  12.24 Ang
40:   1  1       x,       y, -1.00+z    -1.3 kJ/mol  10.69 Ang
41:   1  1       x,       y,  1.00+z    -1.3 kJ/mol  10.69 Ang
42:   1  2 -1.00+x,       y, -1.00+z    -1.2 kJ/mol  10.52 Ang
43:   2  2       x, -1.00+y, -1.00+z    -1.2 kJ/mol  10.92 Ang
44:   2  2       x,  1.00+y,  1.00+z    -1.2 kJ/mol  10.92 Ang
45:   2  1  1.00+x,       y,  1.00+z    -1.2 kJ/mol  10.52 Ang
46:   2  1       x,       y, -1.00+z    -1.0 kJ/mol  10.66 Ang
47:   1  2       x,       y,  1.00+z    -1.0 kJ/mol  10.66 Ang

Sum of above Molecule-Molecule interactions: -612.10 kJ/mol
```

Table A1.8: Tabulated molecule-molecule interaction energies for but-PERY.

```
1:    1  2       x,       y,       z   -82.3 kJ/mol   3.72 Ang
2:    2  1       x, -1.00+y,       z   -82.3 kJ/mol   3.72 Ang
3:    1  2       x,  1.00+y,       z   -82.3 kJ/mol   3.72 Ang
4:    1  1       x,       y, -1.00+z   -47.0 kJ/mol  19.31 Ang
5:    1  1       x,       y,  1.00+z   -47.0 kJ/mol  19.31 Ang
6:    1  1 -0.50-x,  1.00-y, -0.50+z   -22.9 kJ/mol  10.97 Ang
7:    1  1 -0.50-x,  1.00-y,  0.50+z   -22.9 kJ/mol  10.97 Ang
8:    1  1  0.50-x,  1.00-y, -0.50+z   -22.9 kJ/mol  10.97 Ang
9:    1  1  0.50-x,  1.00-y,  0.50+z   -22.9 kJ/mol  10.97 Ang
10:   1  2  0.50-x,      -y,  0.50+z   -13.3 kJ/mol  11.58 Ang
11:   2  1 -0.50-x,      -y, -0.50+z   -13.3 kJ/mol  11.58 Ang
12:   1  2 -0.50-x,      -y,  0.50+z   -13.3 kJ/mol  11.58 Ang
13:   1  2 -0.50-x,  1.00-y, -0.50+z   -13.3 kJ/mol  11.58 Ang
14:   2  1 -0.50-x,  1.00-y,  0.50+z   -13.3 kJ/mol  11.58 Ang
15:   2  1  0.50-x,      -y, -0.50+z   -13.3 kJ/mol  11.58 Ang
16:   1  2  0.50-x,  1.00-y, -0.50+z   -13.3 kJ/mol  11.58 Ang
17:   2  1  0.50-x,  1.00-y,  0.50+z   -13.3 kJ/mol  11.58 Ang
18:   2  1  0.50-x,      -y,  0.50+z    -7.8 kJ/mol  11.58 Ang
19:   1  2 -0.50-x,      -y, -0.50+z    -7.8 kJ/mol  11.58 Ang
20:   2  1 -0.50-x,      -y,  0.50+z    -7.8 kJ/mol  11.58 Ang
21:   2  1 -0.50-x,  1.00-y, -0.50+z    -7.8 kJ/mol  11.58 Ang
22:   1  2 -0.50-x,  1.00-y,  0.50+z    -7.8 kJ/mol  11.58 Ang
23:   1  2  0.50-x,      -y, -0.50+z    -7.8 kJ/mol  11.58 Ang
24:   2  1  0.50-x,  1.00-y, -0.50+z    -7.8 kJ/mol  11.58 Ang
25:   1  2  0.50-x,  1.00-y,  0.50+z    -7.8 kJ/mol  11.58 Ang
26:   1  1       x, -1.00+y,       z    -7.0 kJ/mol   7.45 Ang
27:   1  1       x,  1.00+y,       z    -7.0 kJ/mol   7.45 Ang
28:   2  2       x, -1.00+y,       z    -5.2 kJ/mol   7.45 Ang
29:   2  2       x,  1.00+y,       z    -5.2 kJ/mol   7.45 Ang
30:   2  2  0.50-x,      -y,  0.50+z    -5.0 kJ/mol  10.97 Ang
31:   2  2 -0.50-x,      -y, -0.50+z    -5.0 kJ/mol  10.97 Ang
32:   2  2 -0.50-x,      -y,  0.50+z    -5.0 kJ/mol  10.97 Ang
33:   2  2  0.50-x,      -y, -0.50+z    -5.0 kJ/mol  10.97 Ang
34:   2  2 -1.00+x,       y,       z    -3.5 kJ/mol  10.40 Ang
35:   2  2  1.00+x,       y,       z    -3.5 kJ/mol  10.40 Ang
```

```
36:   1  1       x, -1.00+y,  1.00+z    -2.2 kJ/mol  20.70 Ang
37:   1  1       x,  1.00+y, -1.00+z    -2.2 kJ/mol  20.70 Ang
38:   1  1  0.50-x,      -y,  0.50+z    -1.6 kJ/mol  13.26 Ang
39:   1  1 -0.50-x,      -y, -0.50+z    -1.6 kJ/mol  13.26 Ang
40:   1  1 -1.00+x,       y,       z    -1.6 kJ/mol  10.40 Ang
41:   1  1 -0.50-x,      -y,  0.50+z    -1.6 kJ/mol  13.26 Ang
42:   1  1 -0.50-x,  2.00-y, -0.50+z    -1.6 kJ/mol  13.26 Ang
43:   1  1 -0.50-x,  2.00-y,  0.50+z    -1.6 kJ/mol  13.26 Ang
44:   1  1  0.50-x,      -y, -0.50+z    -1.6 kJ/mol  13.26 Ang
45:   1  1  0.50-x,  2.00-y, -0.50+z    -1.6 kJ/mol  13.26 Ang
46:   1  1  0.50-x,  2.00-y,  0.50+z    -1.6 kJ/mol  13.26 Ang
47:   1  1  1.00+x,       y,       z    -1.6 kJ/mol  10.40 Ang
48:   2  1 -1.00+x, -1.00+y,       z    -1.2 kJ/mol  11.04 Ang
49:   1  2 -1.00+x,       y,       z    -1.2 kJ/mol  11.04 Ang
50:   2  1 -1.00+x,       y,       z    -1.2 kJ/mol  11.04 Ang
51:   1  2 -1.00+x,  1.00+y,       z    -1.2 kJ/mol  11.04 Ang
52:   2  1  1.00+x, -1.00+y,       z    -1.2 kJ/mol  11.04 Ang
53:   1  2  1.00+x,       y,       z    -1.2 kJ/mol  11.04 Ang
54:   2  1  1.00+x,       y,       z    -1.2 kJ/mol  11.04 Ang
55:   1  2  1.00+x,  1.00+y,       z    -1.2 kJ/mol  11.04 Ang

Sum of above Molecule-Molecule interactions: -682.70 kJ/mol
```

Appendix: A2 – PXRD Patterns

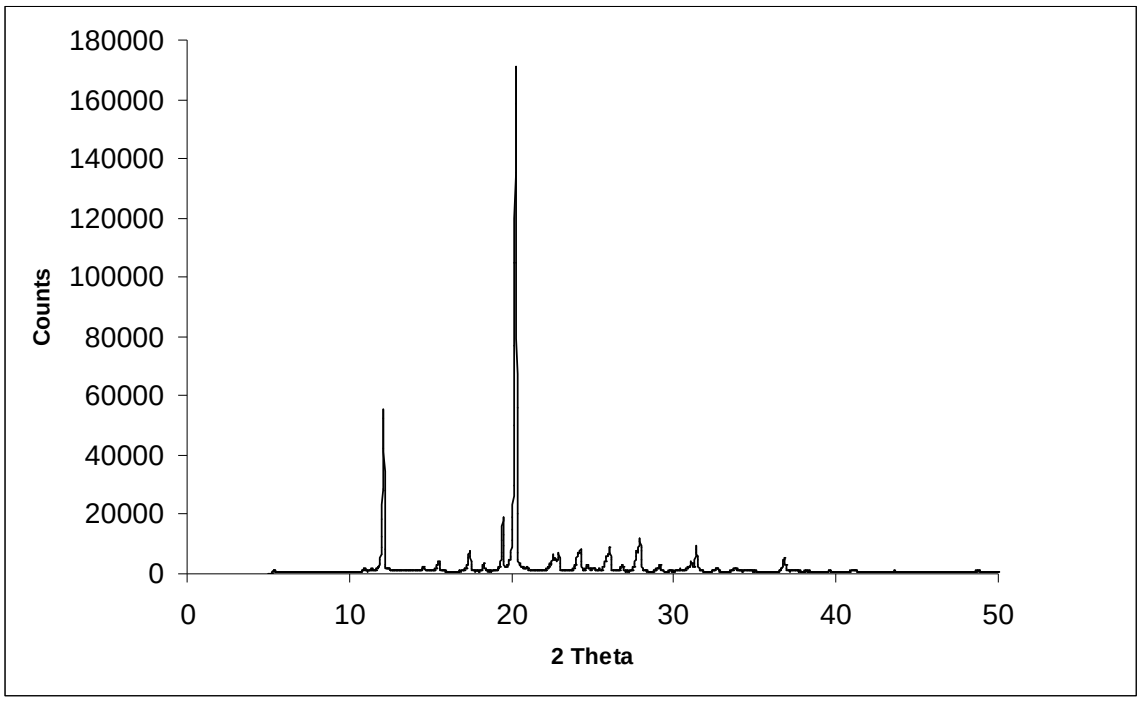


Figure A2.1: PXRD for gly-L.

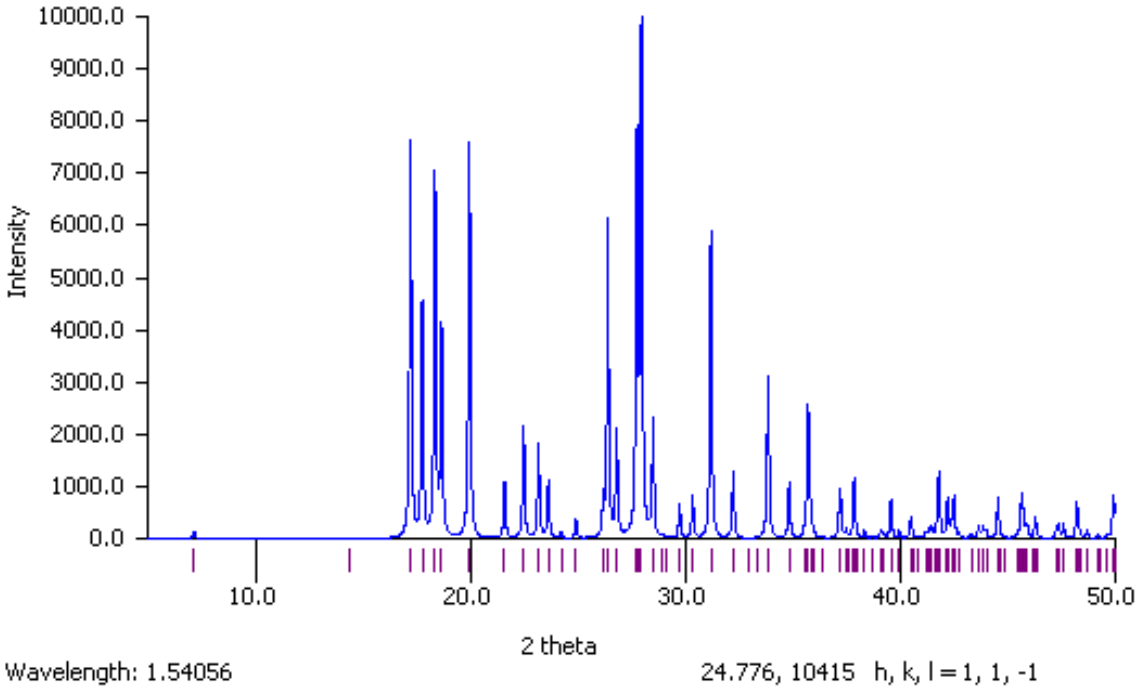


Figure A2.2: Calculated PXRD for gly-L.

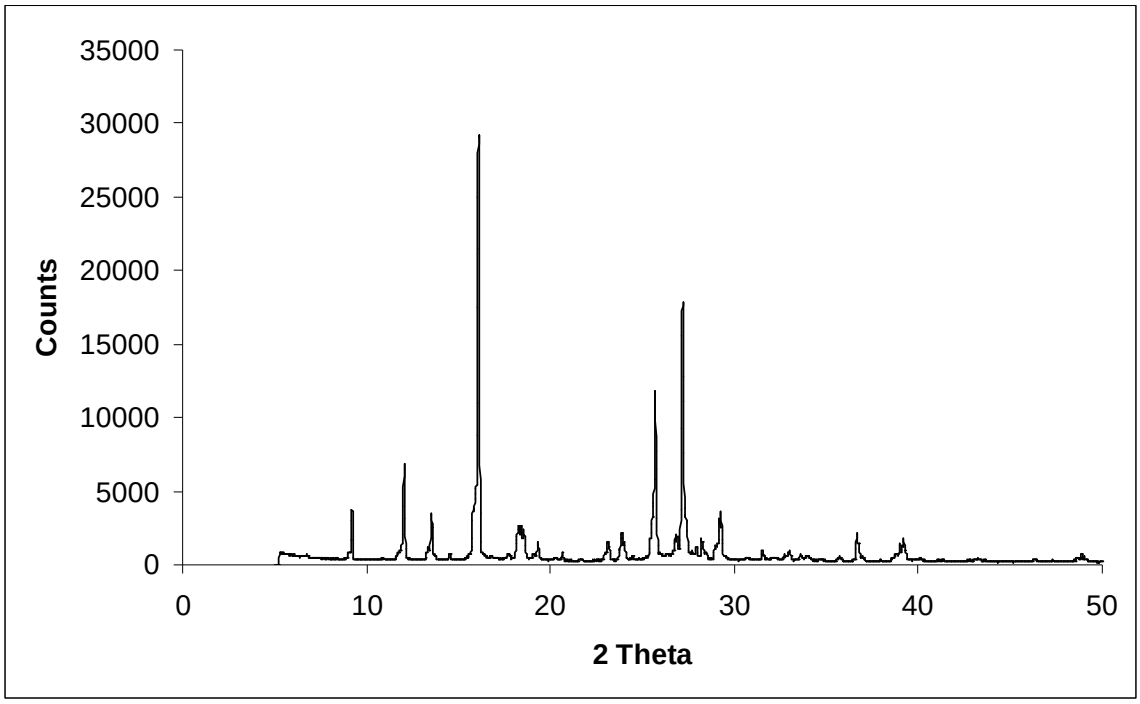


Figure A2.3: PXRD for gly-NAP.

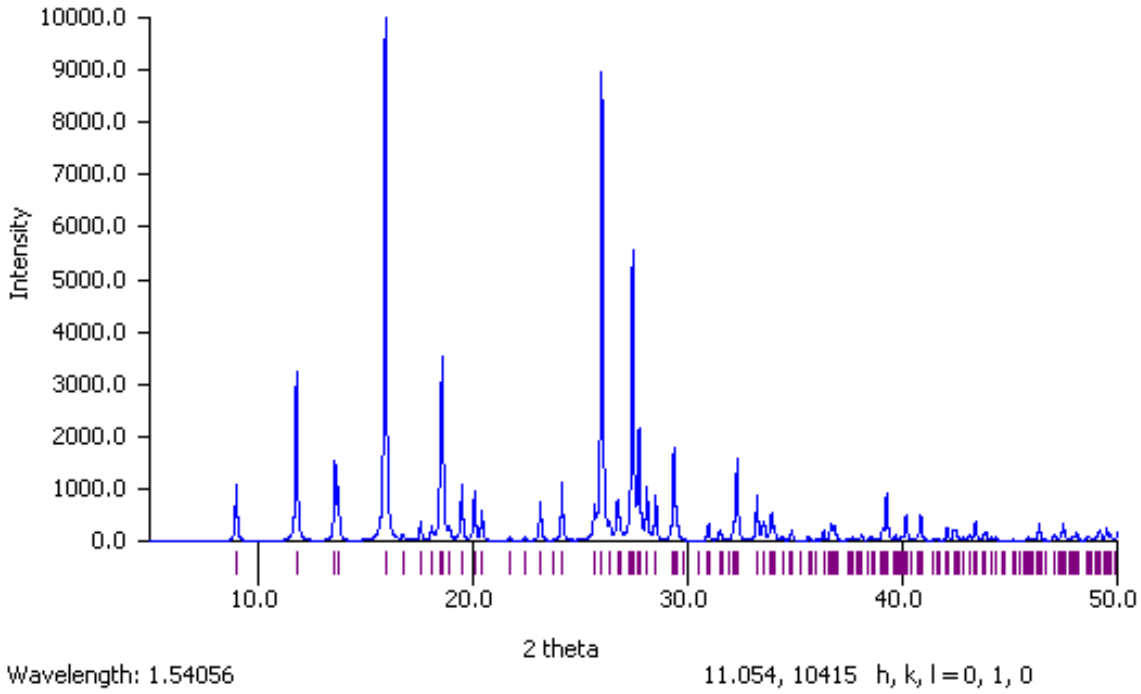


Figure A2.4: Calculated PXRD for gly-NAP.

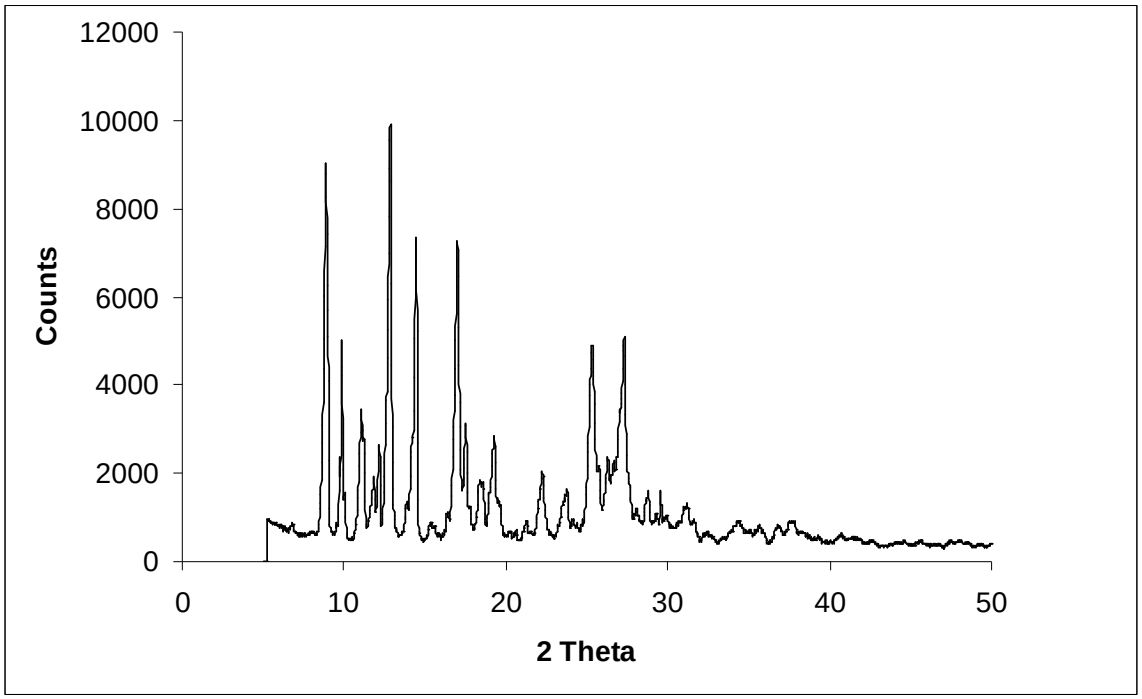


Figure A2.5: PXRD for gly-ANT.

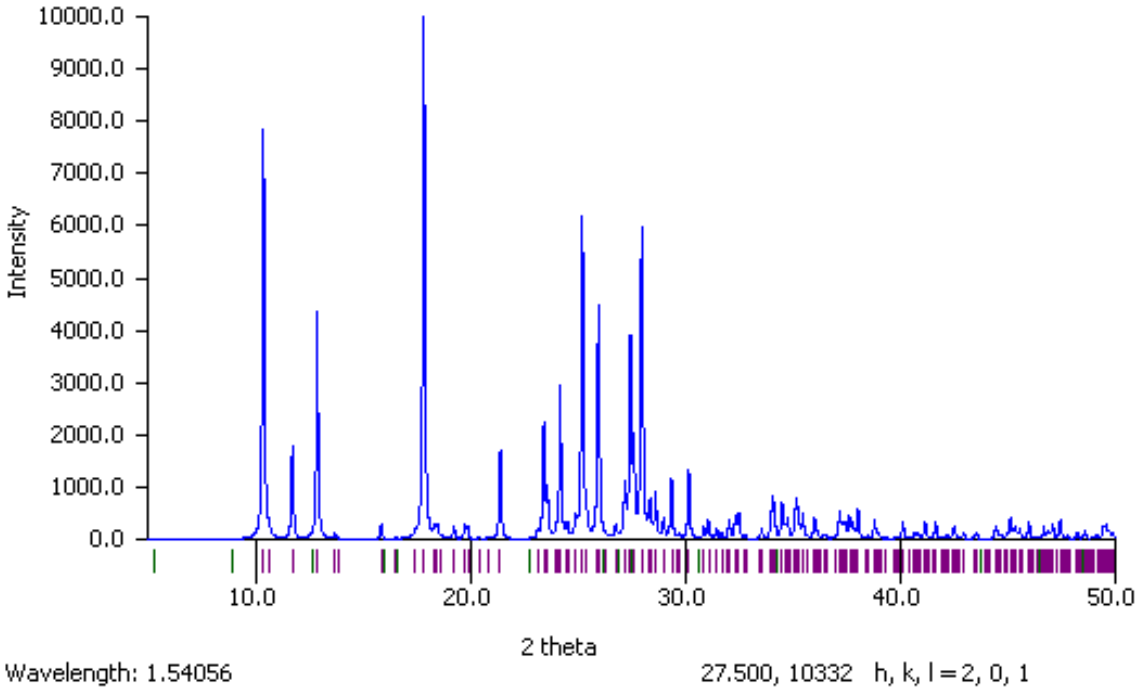


Figure A2.6: Calculated PXRD for gly-ANT.

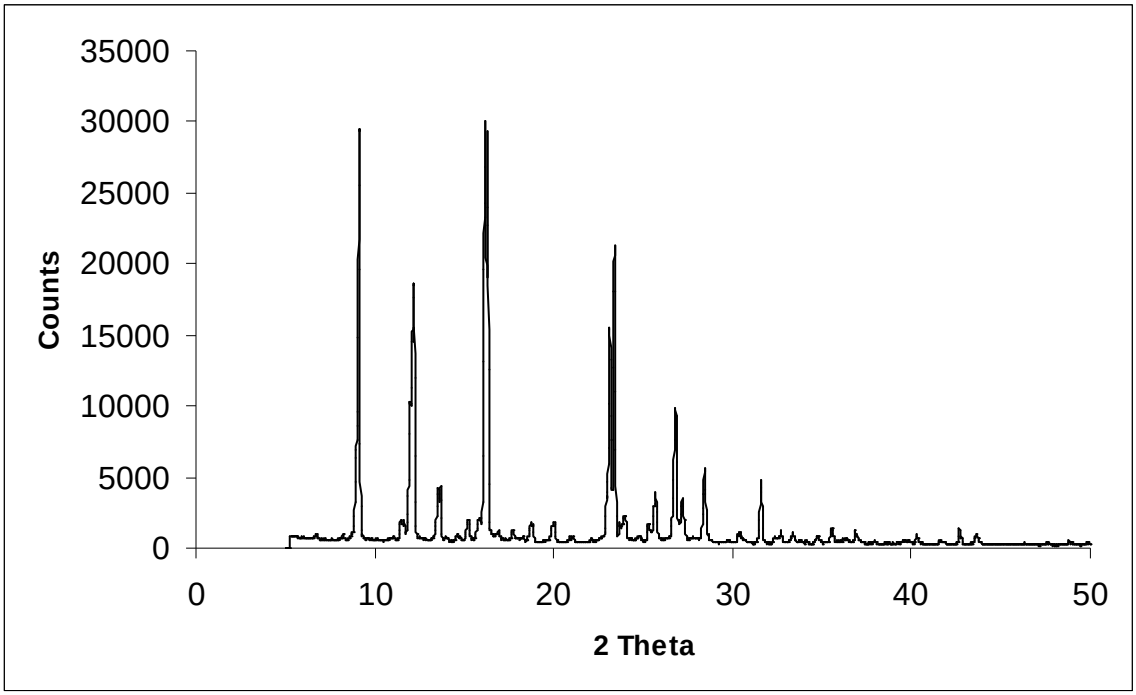


Figure A2.7: PXRD for gly-PHEN.

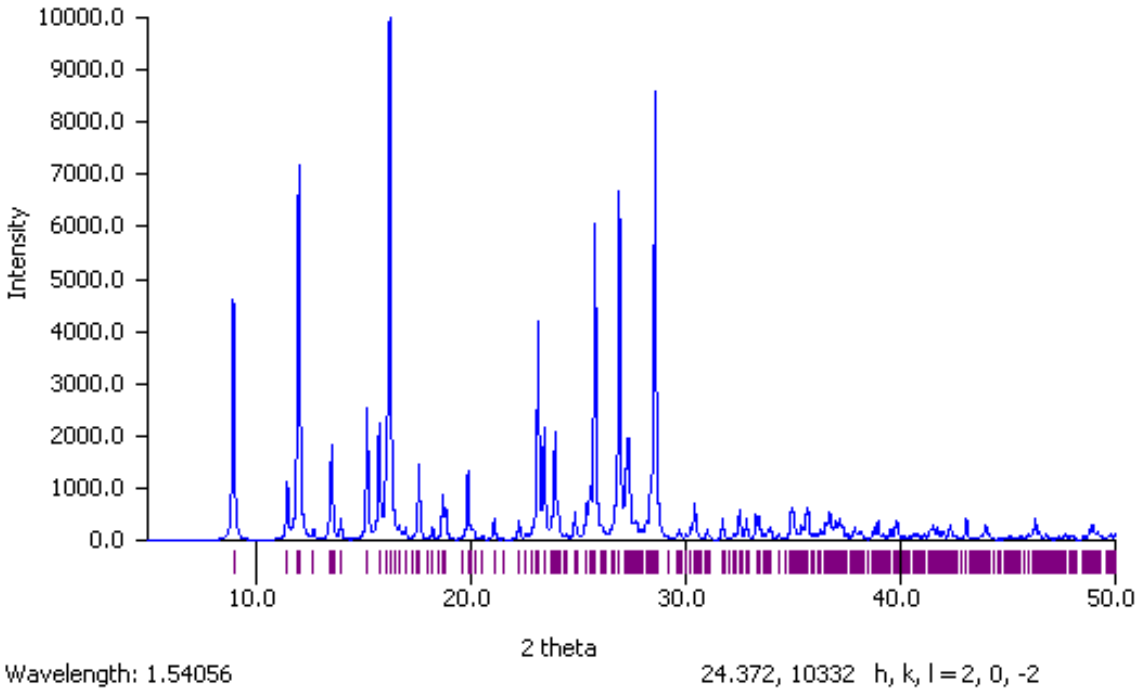


Figure A2.8: Calculated PXRD for gly-PHEN.

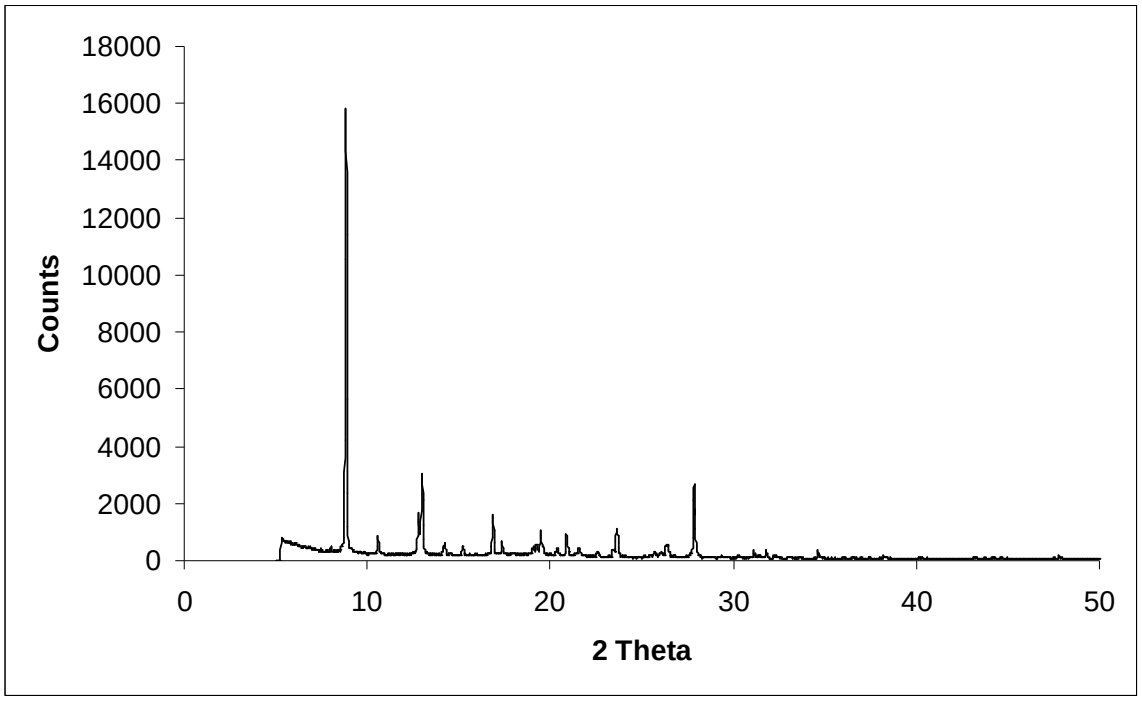


Figure A2.9: PXRD for gly-PERY.

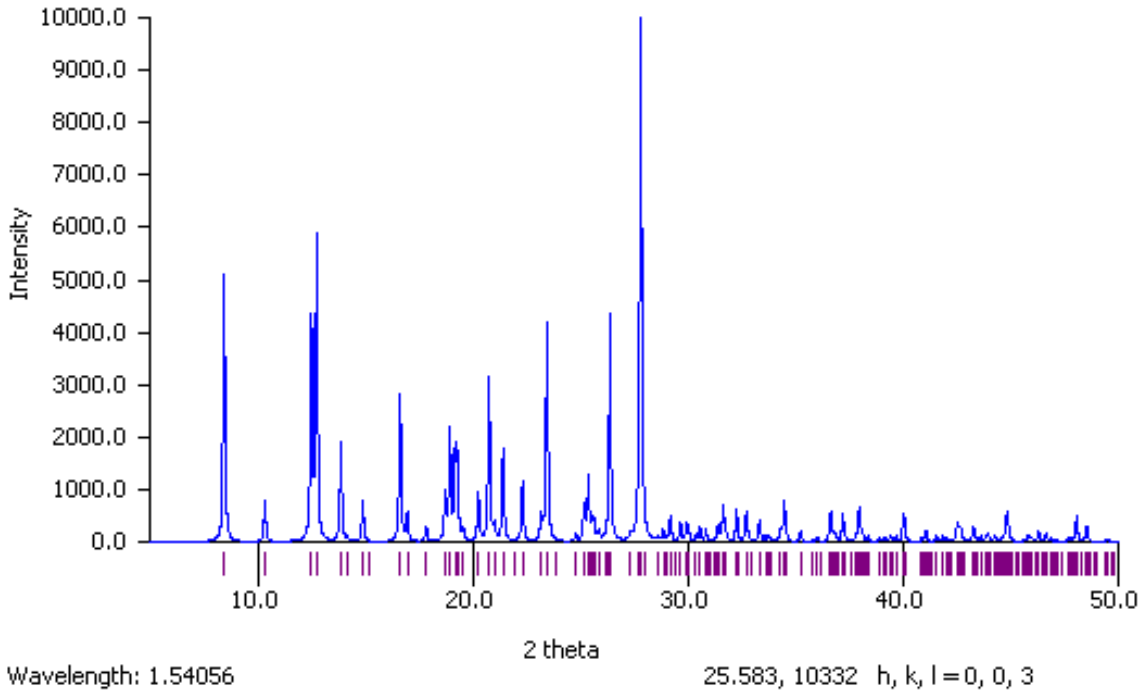


Figure A2.10: Calculated PXRD for gly-PERY.

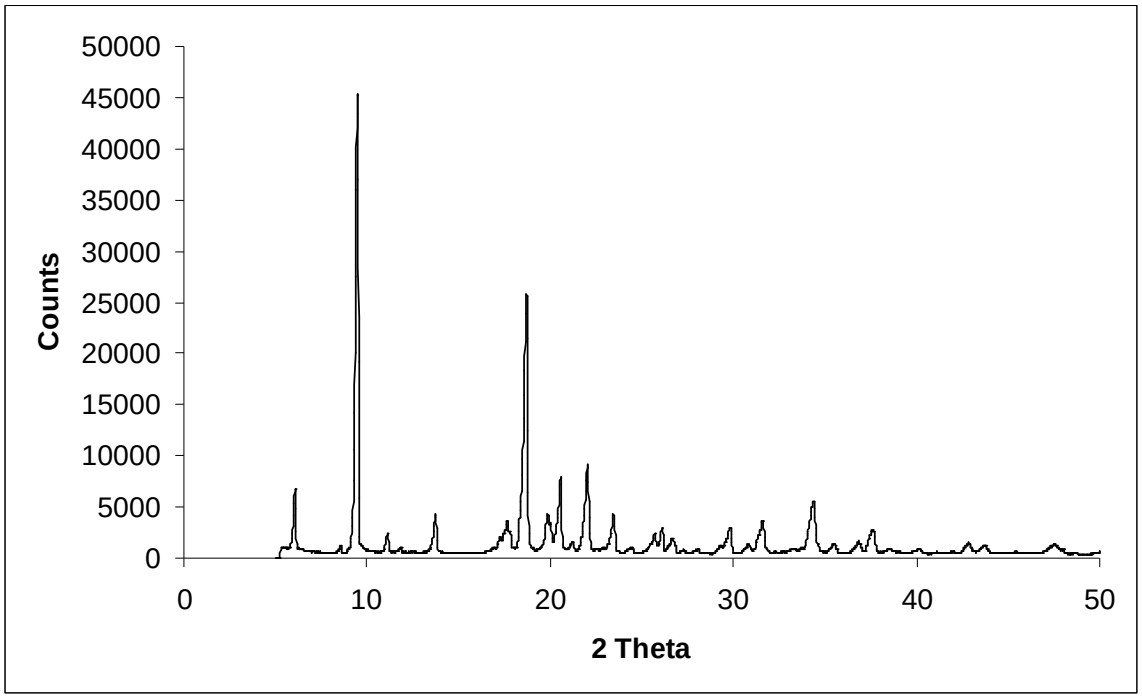


Figure A2.11: PXRD for but-L.

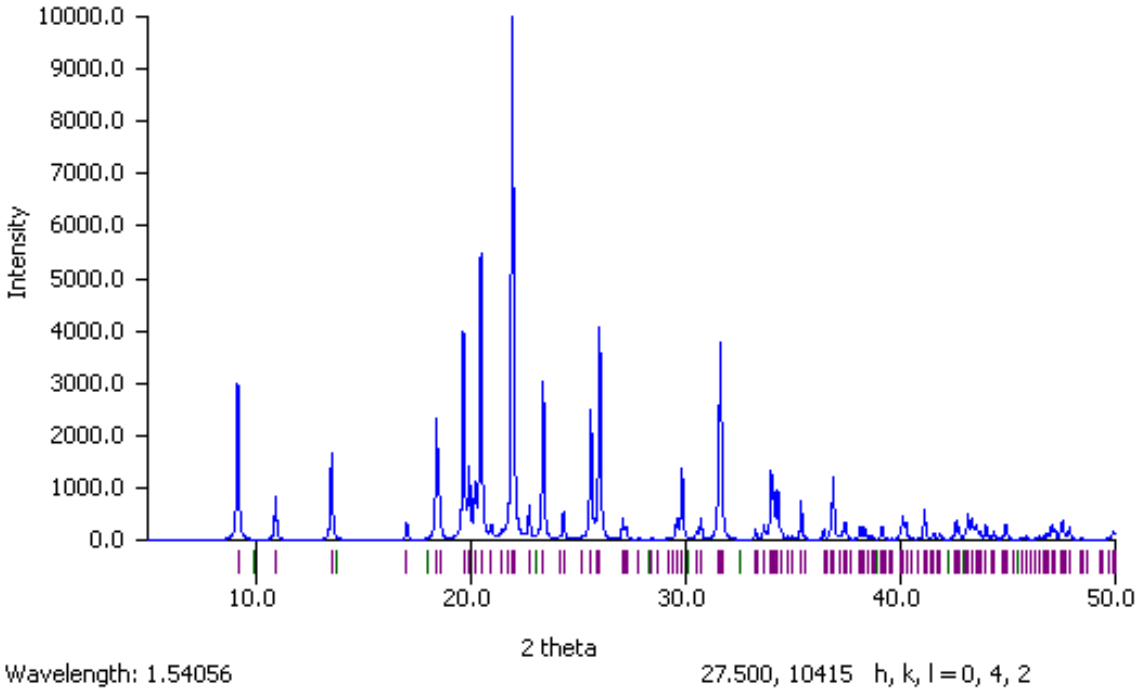


Figure A2.12: Calculated PXRD for but-L.

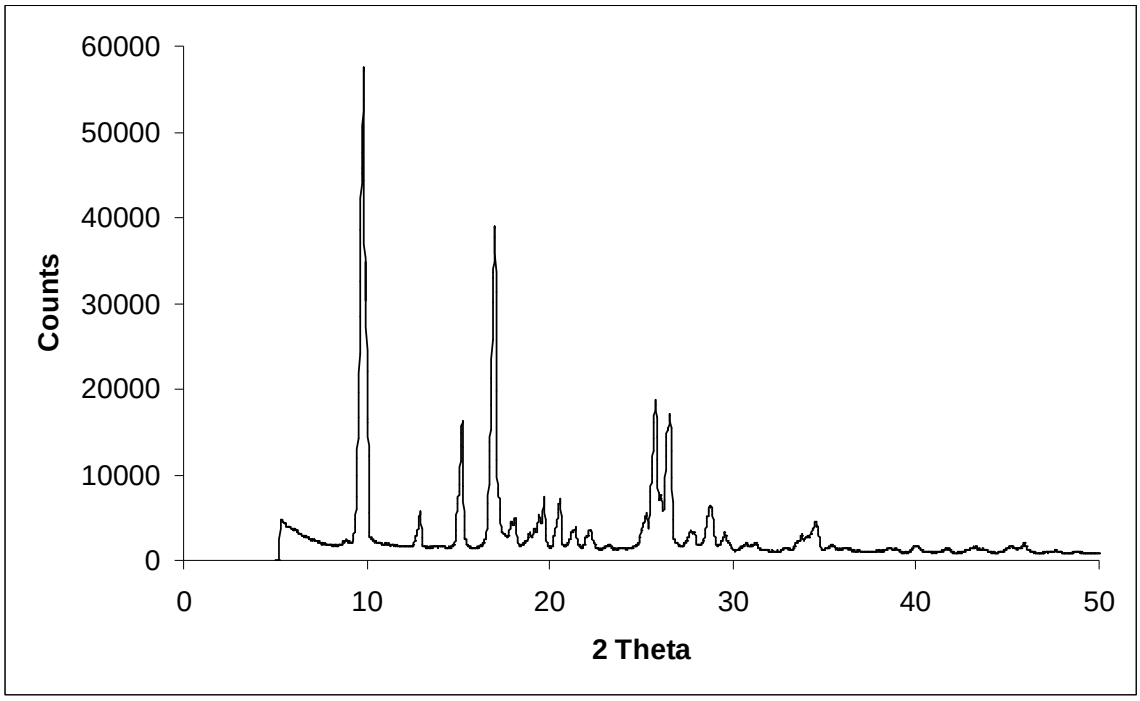


Figure A2.13: PXRD for but-PHEN.

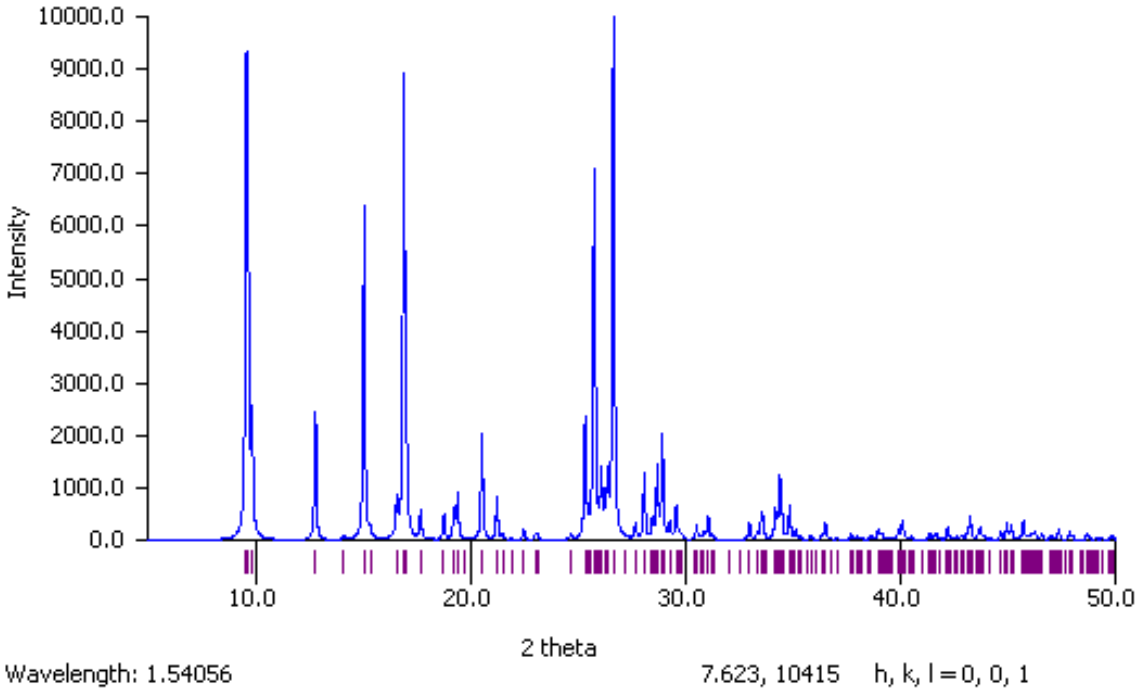


Figure A2.14: Calculated PXRD for but-PHEN.

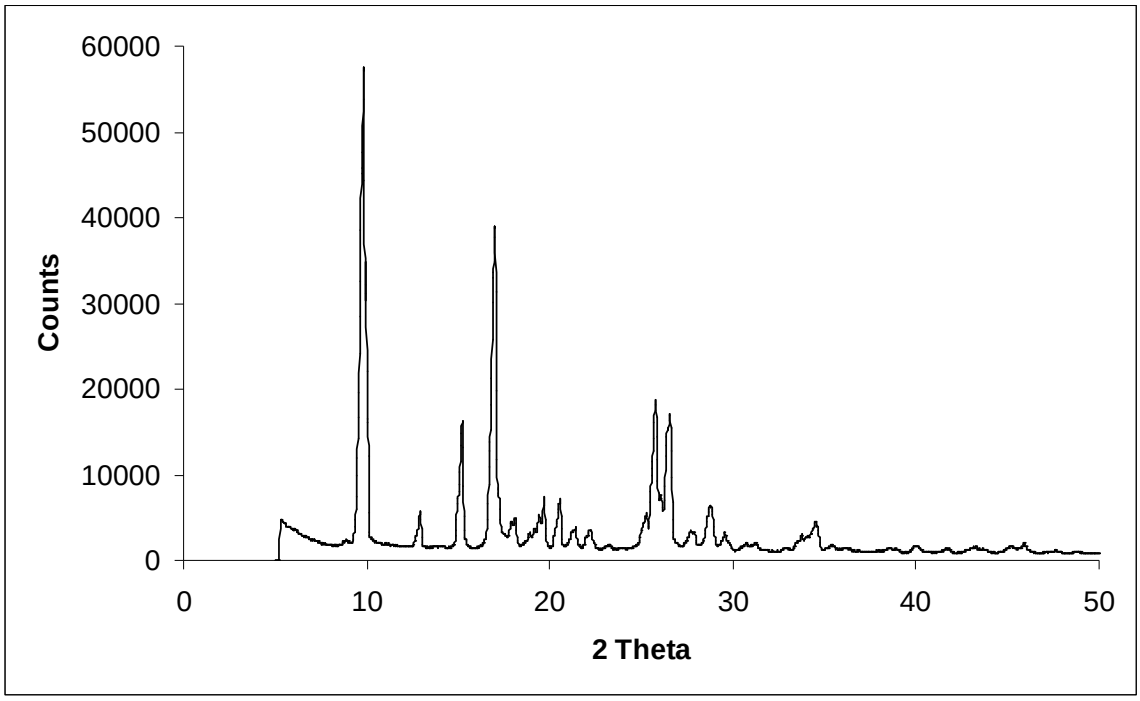


Figure A2.15: PXRD for but-PERY.

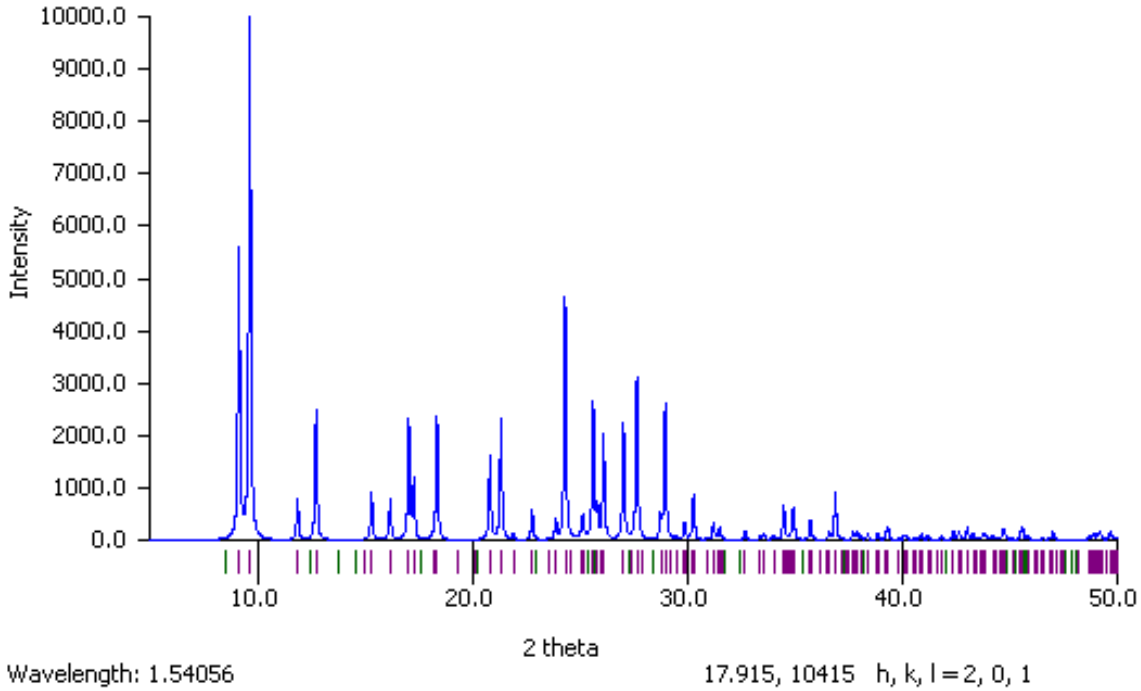


Figure A2.16: Calculated PXRD for but-PERY.

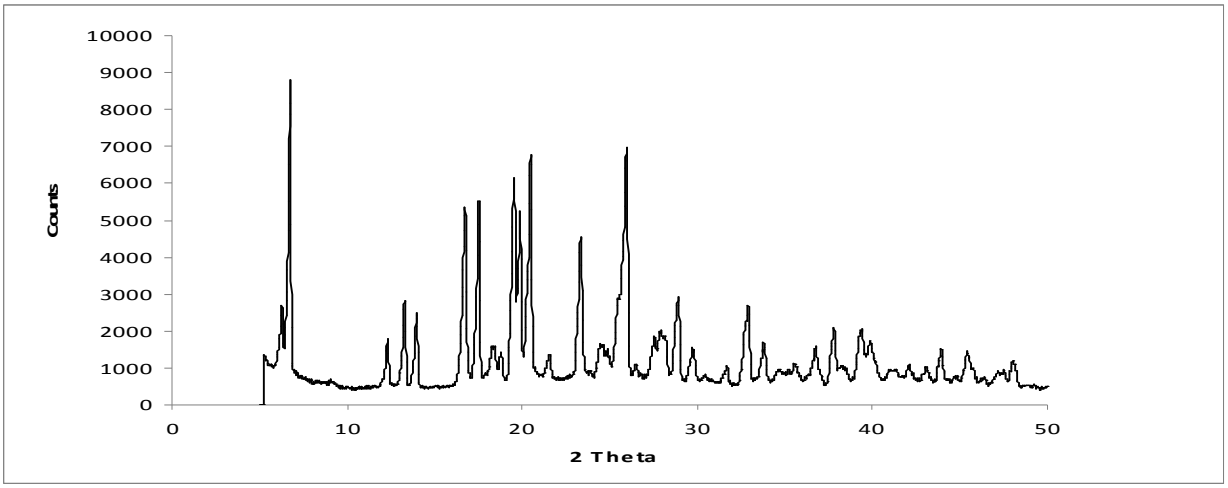


Figure A2.17: PXRD for MOF-Zn.

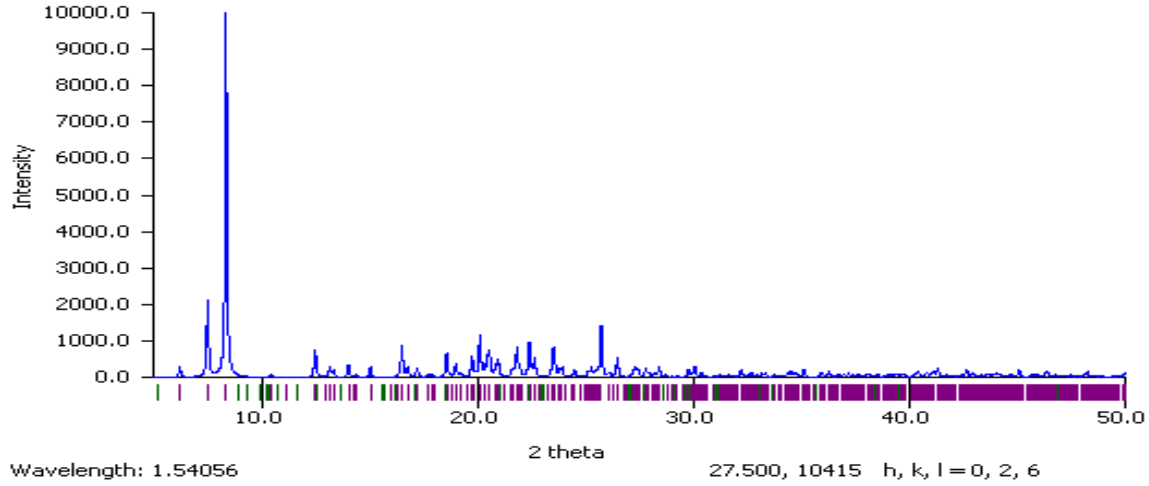


Figure A2.18: Calculated PXRD for MOF-Zn1.

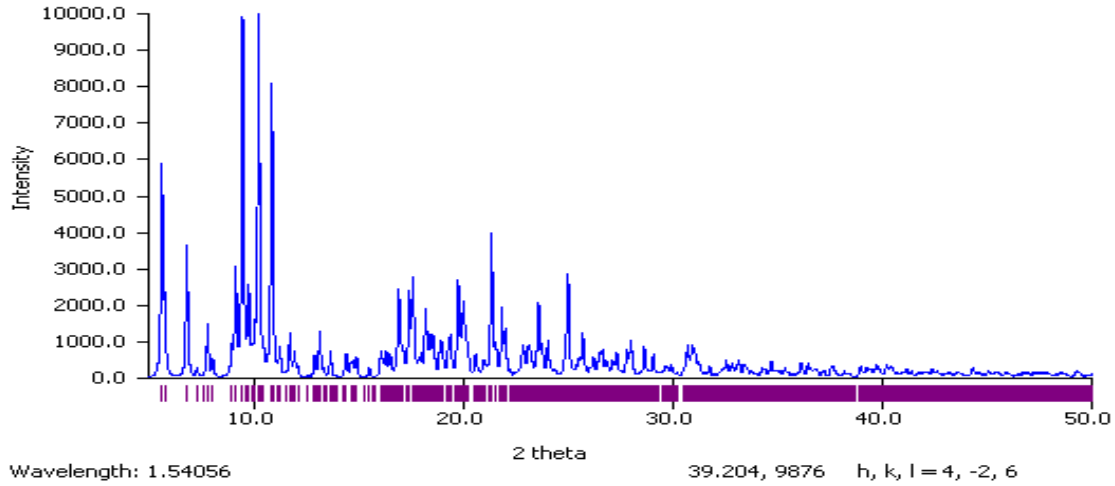


Figure A2.19: Calculated PXRD for MOF-Zn2.

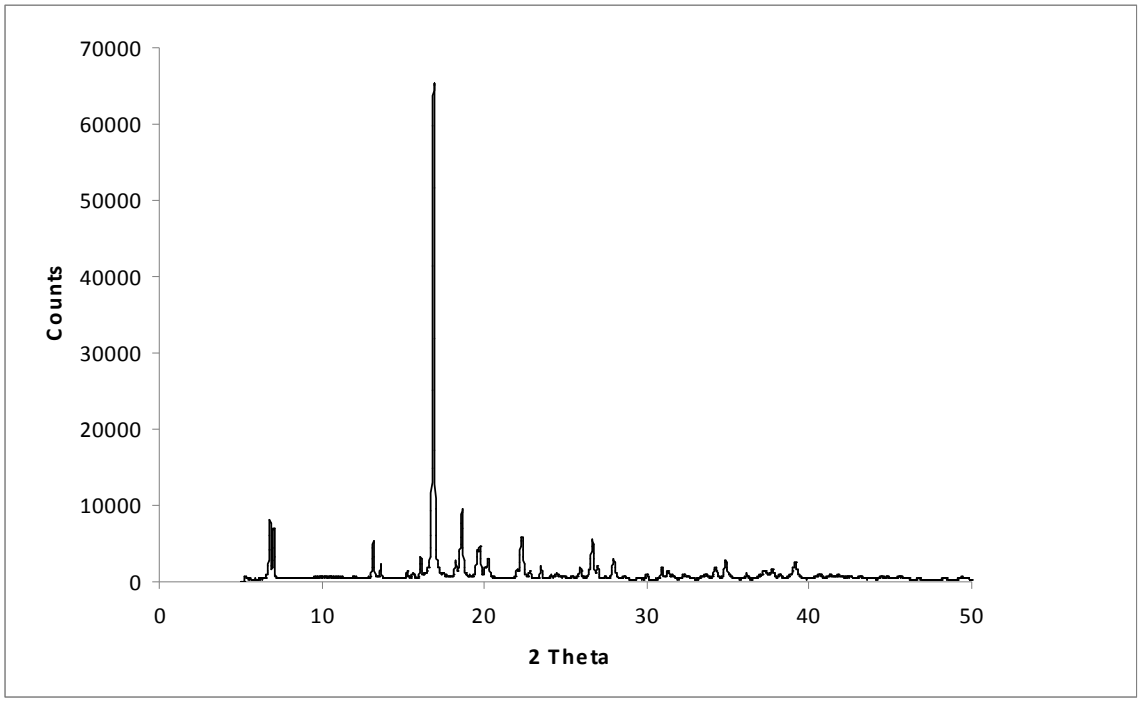


Figure A2.20: PXRD for MOF-Cd1.

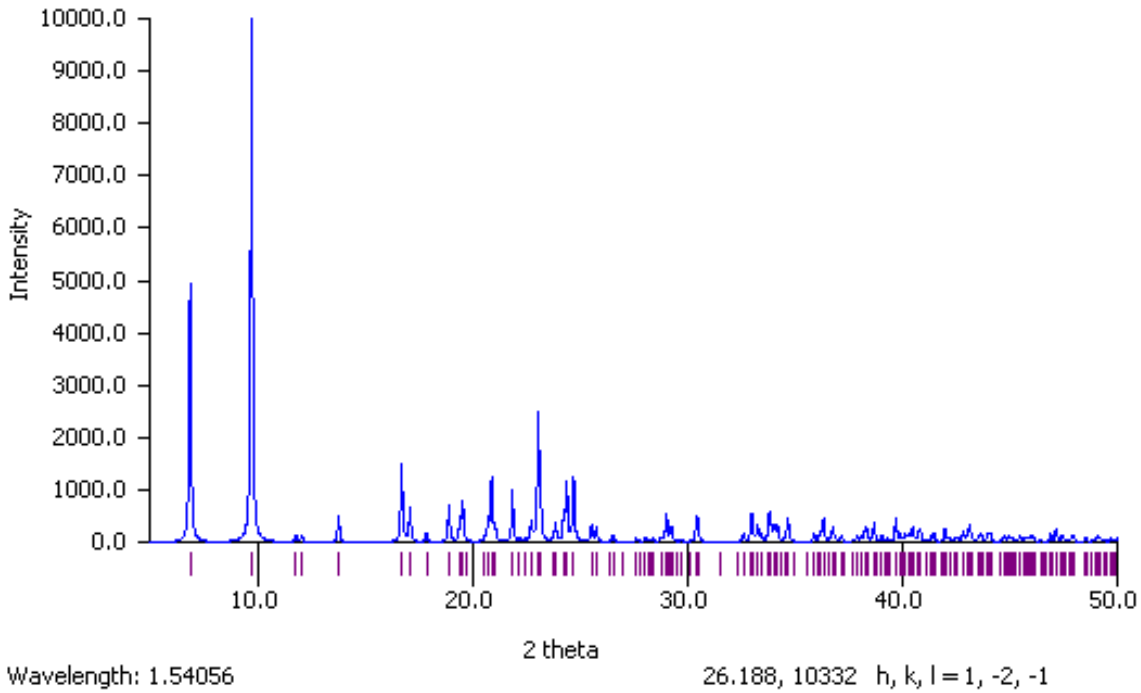


Figure A2.21: Calculated PXRD for MOF-Cd1.

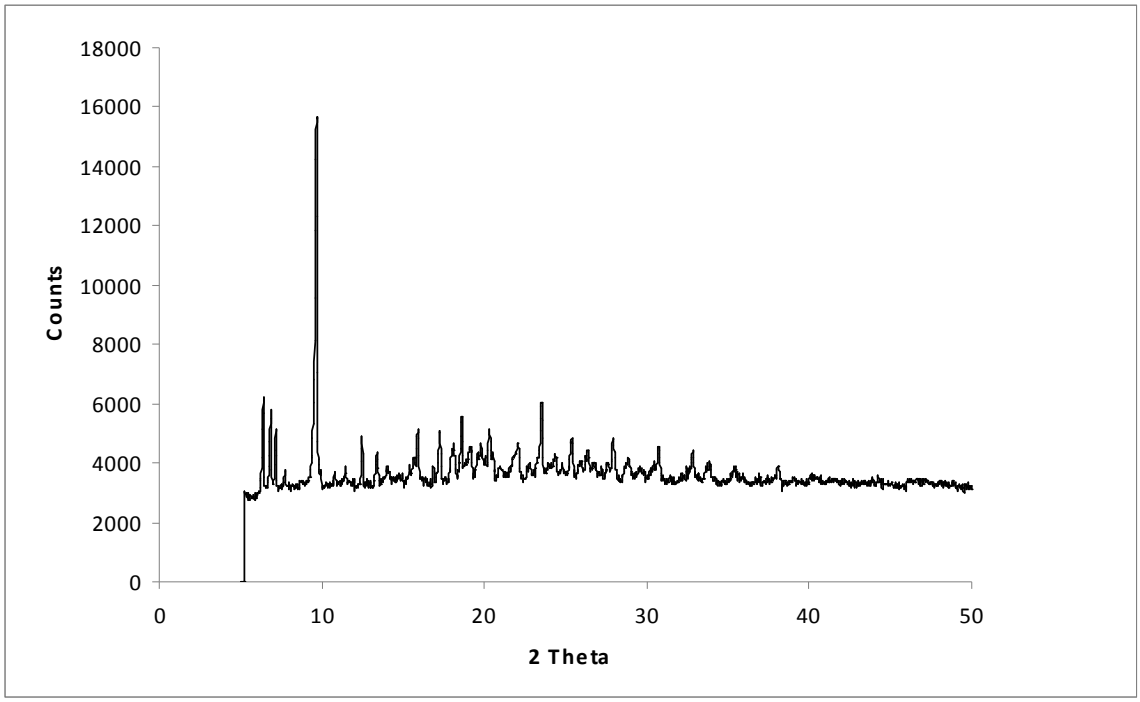


Figure A2.22: PXRD for MOF-Co1.

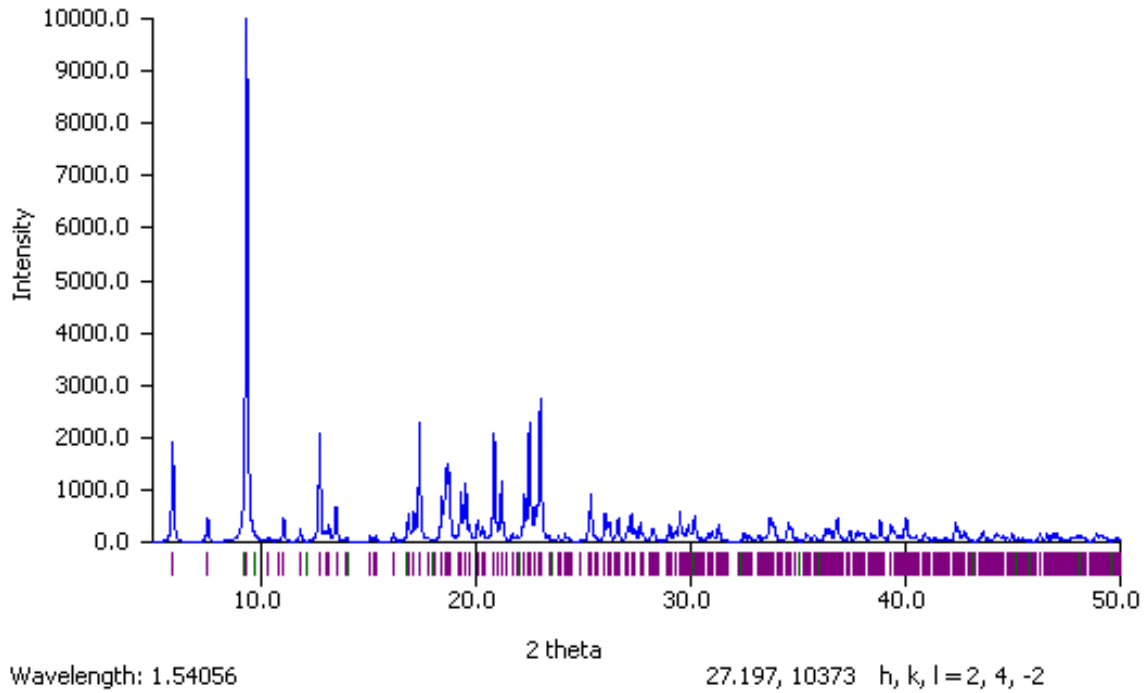


Figure A2.23: Calculated PXRD for MOF-Co1.

Appendix: A3 - Thermal Data

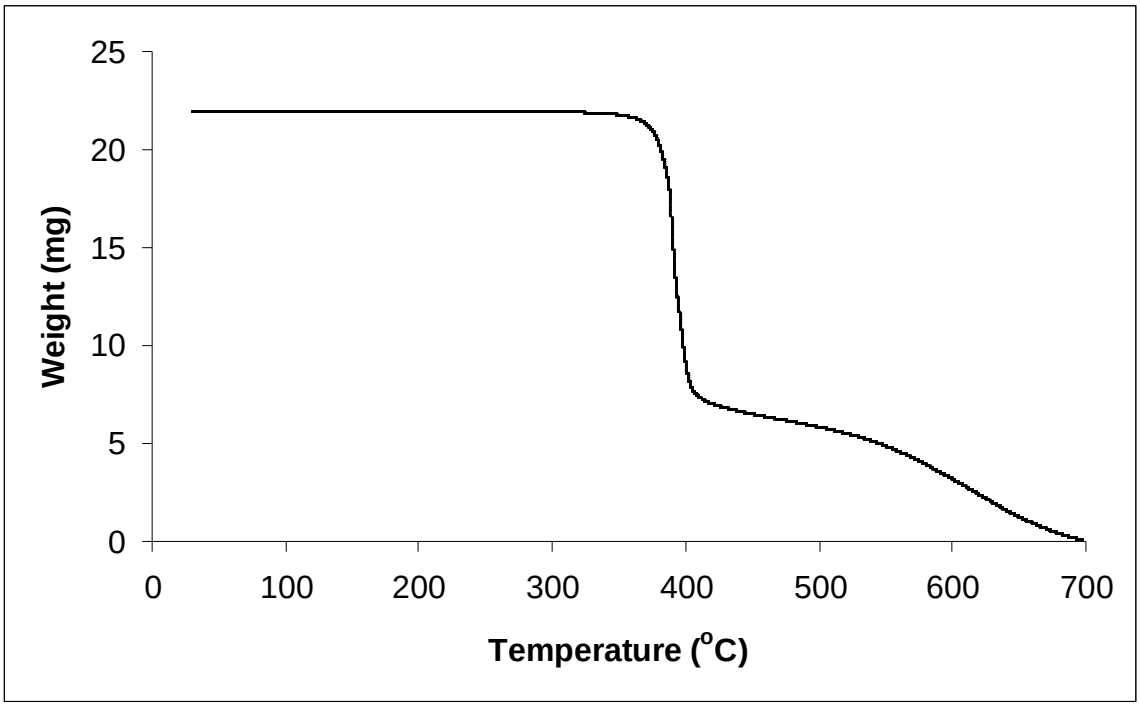


Figure A3.1: Thermogravimetric trace for gly-L.

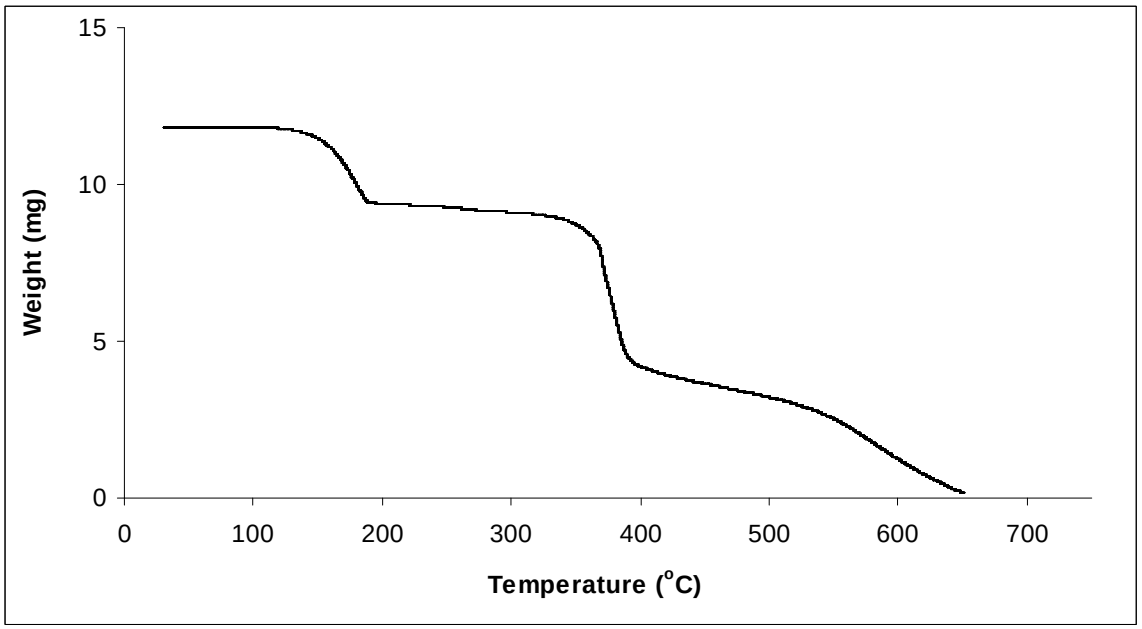


Figure A3.2: Thermogravimetric trace for gly-NAP.

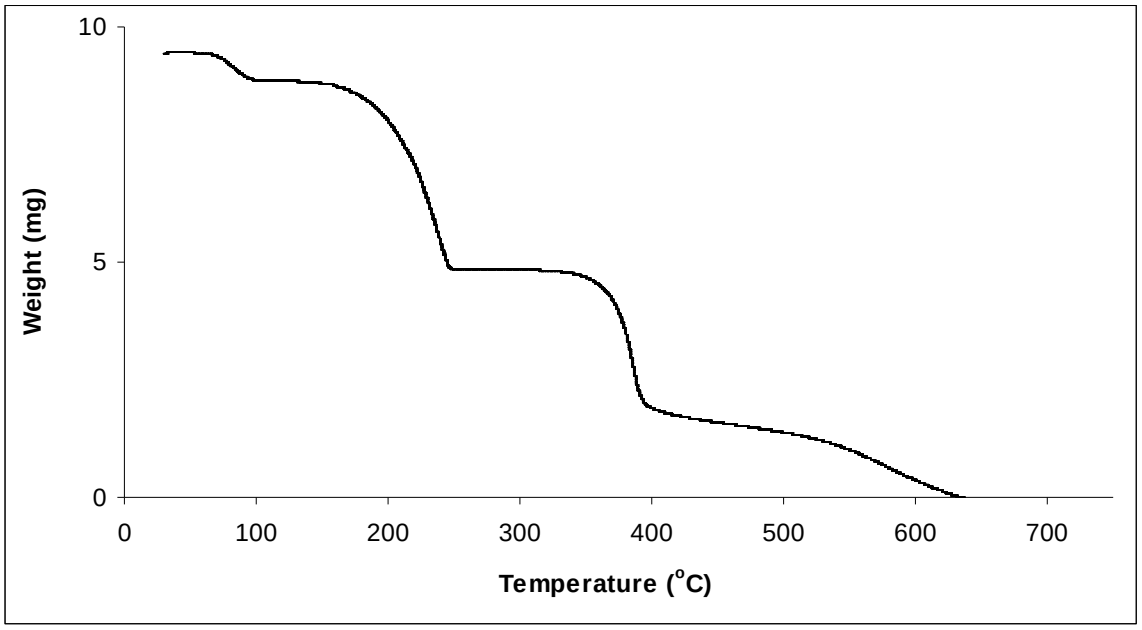


Figure A3.3: Thermogravimetric trace for gly-ANT.

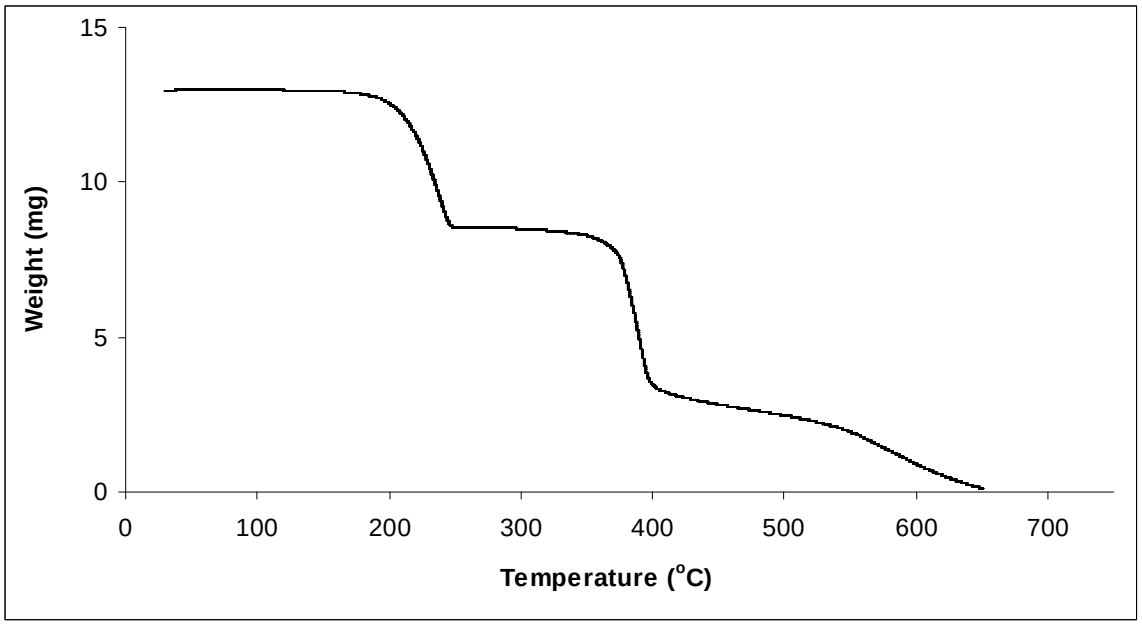


Figure A3.4: Thermogravimetric trace for gly-PHEN.

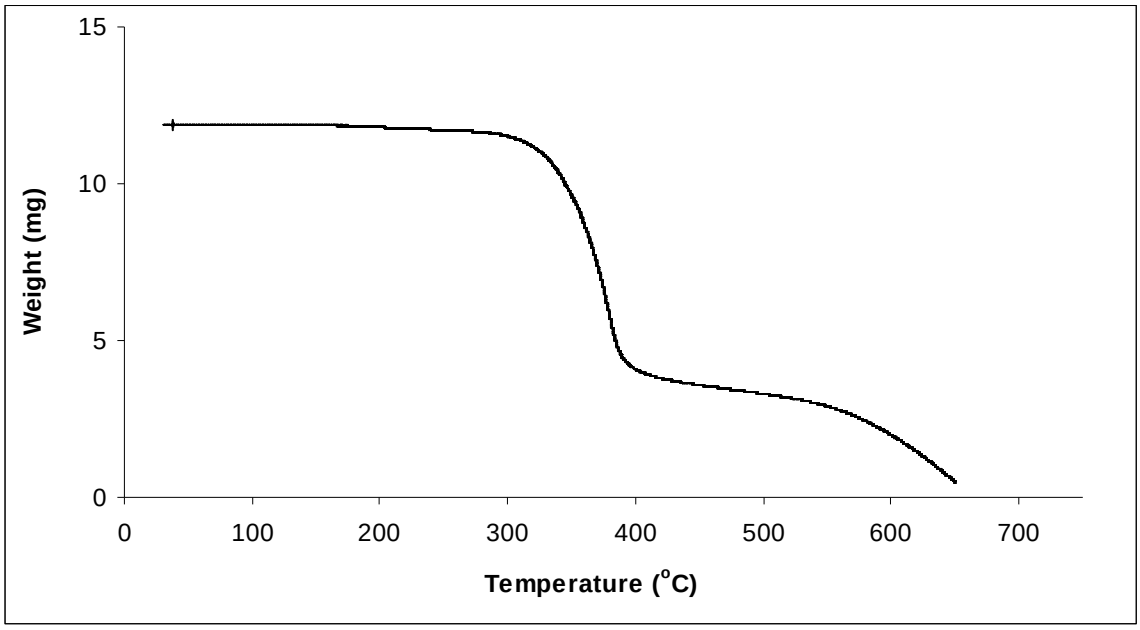


Figure A3.5: Thermogravimetric trace for gly-PERY.

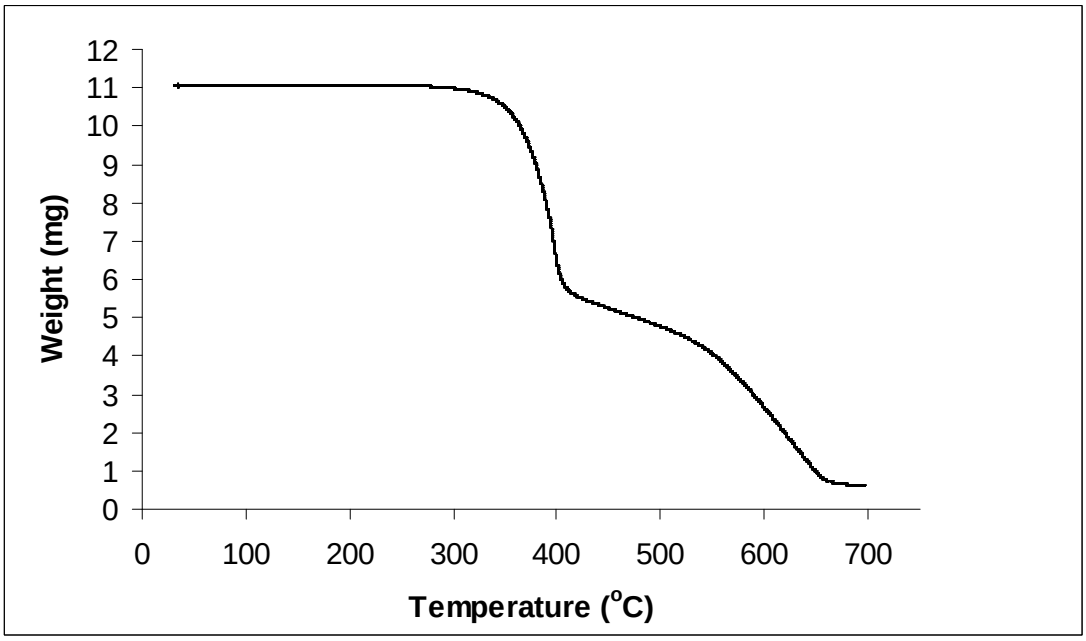


Figure A3.6: Thermogravimetric trace for but-L.

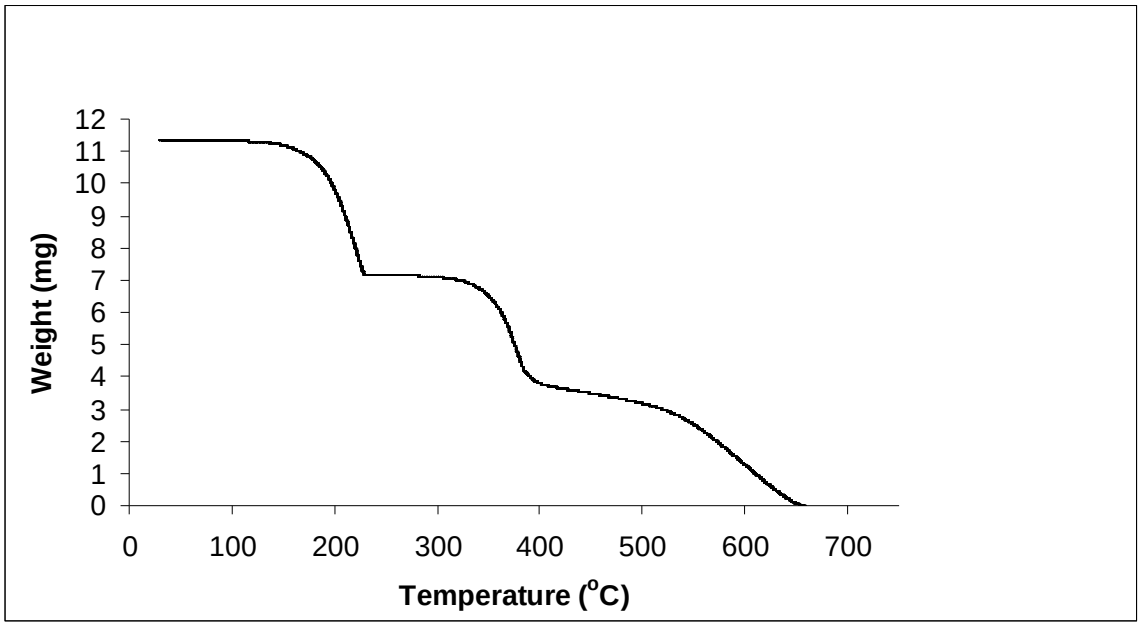


Figure A3.7: Thermogravimetric trace for but-PHEN.

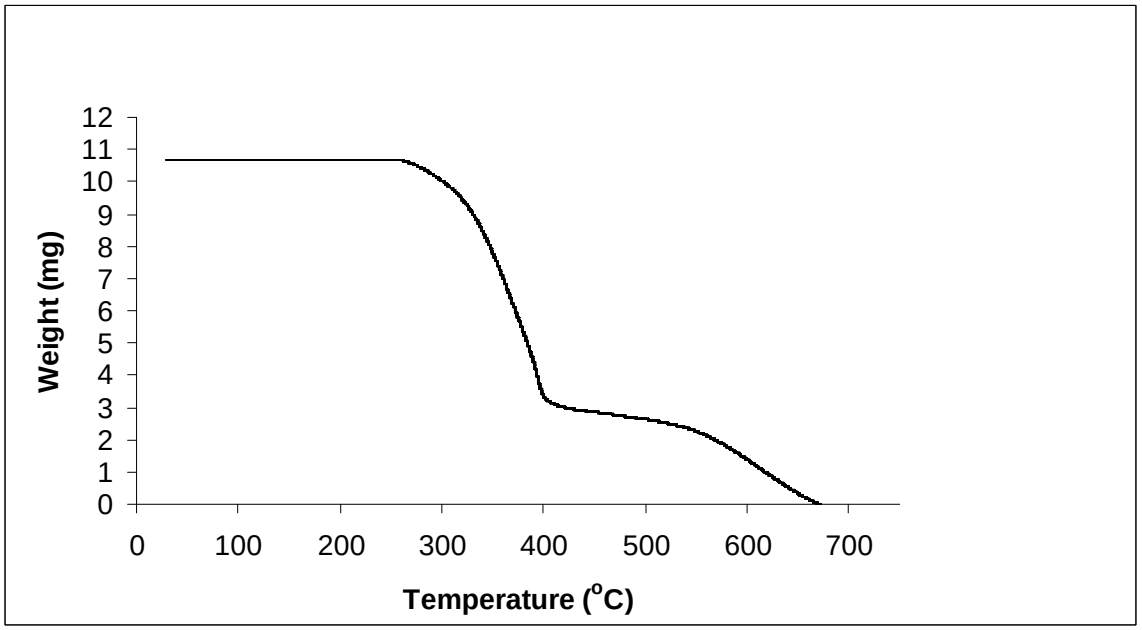


Figure A3.8: Thermogravimetric trace for but-PERY.

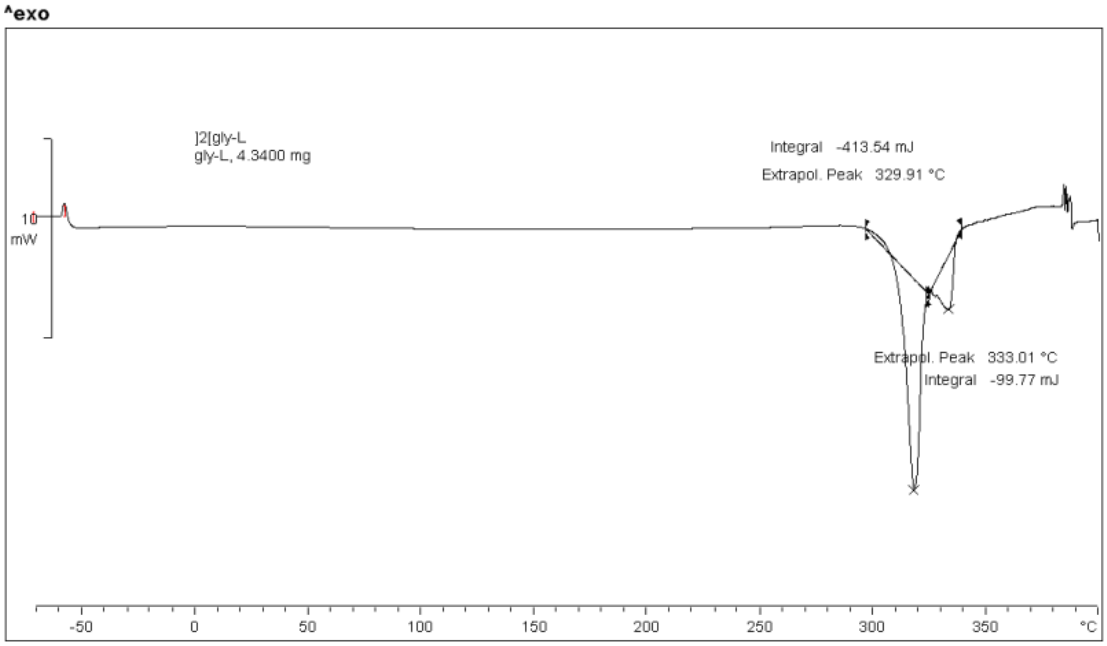


Figure A3.9: DSC curves of heat flow (mW) vs. temperature (^{o}C) for gly-L.

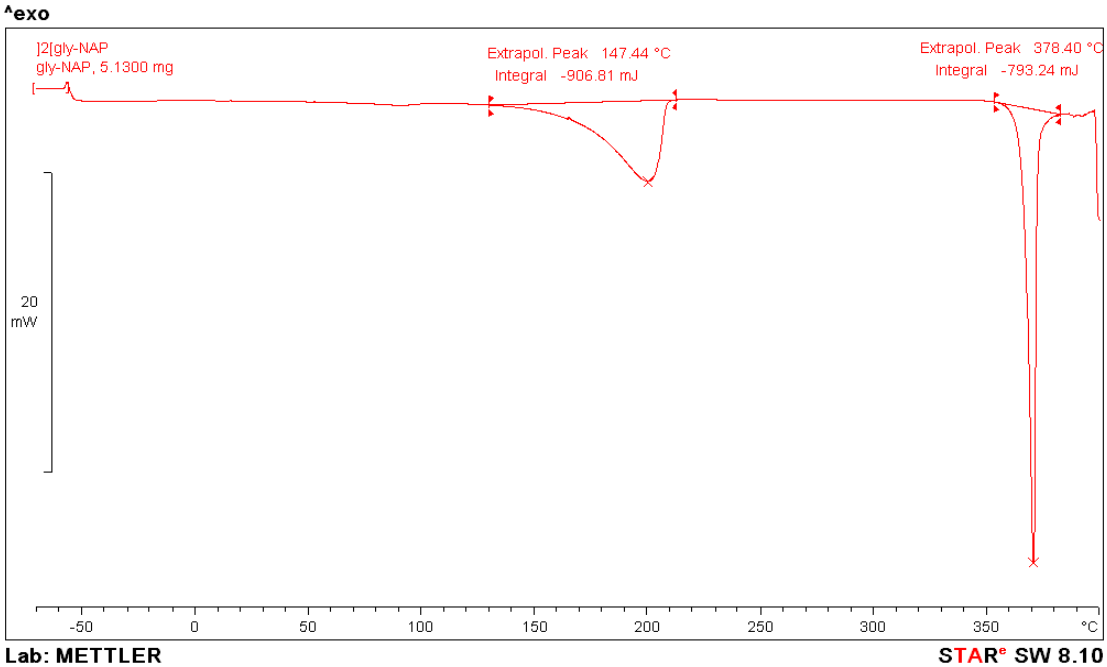


Figure A3.10: DSC curves of heat flow (mW) vs. temperature (^{o}C) for gly-NAP.

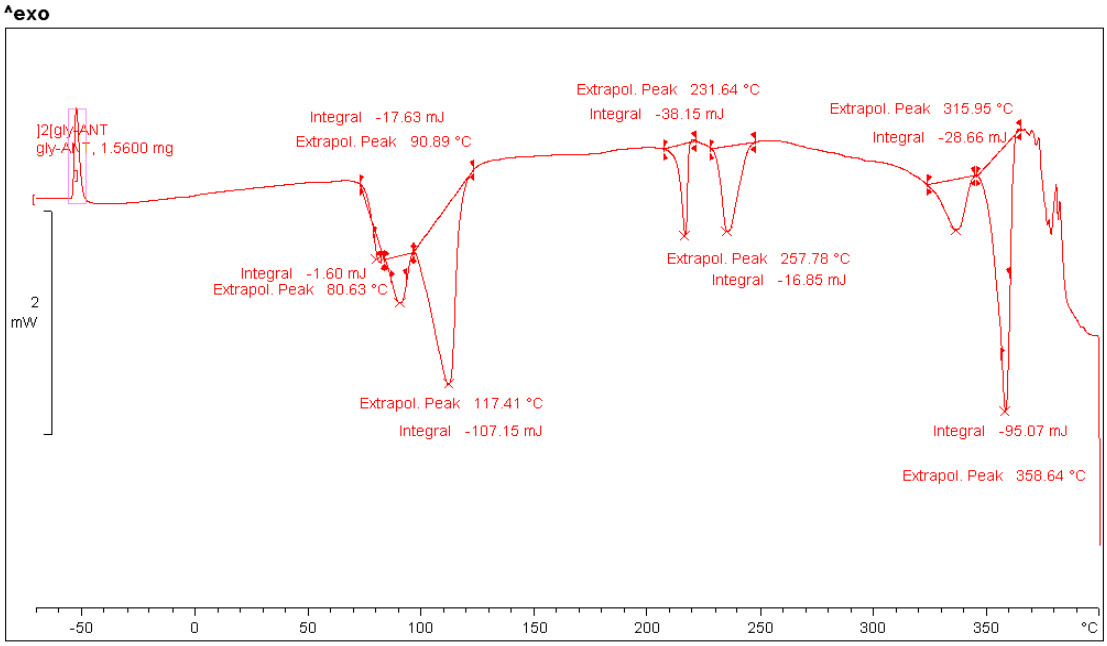


Figure A3.11: DSC curves of heat flow (mW) vs. temperature (^{o}C) for gly-ANT.

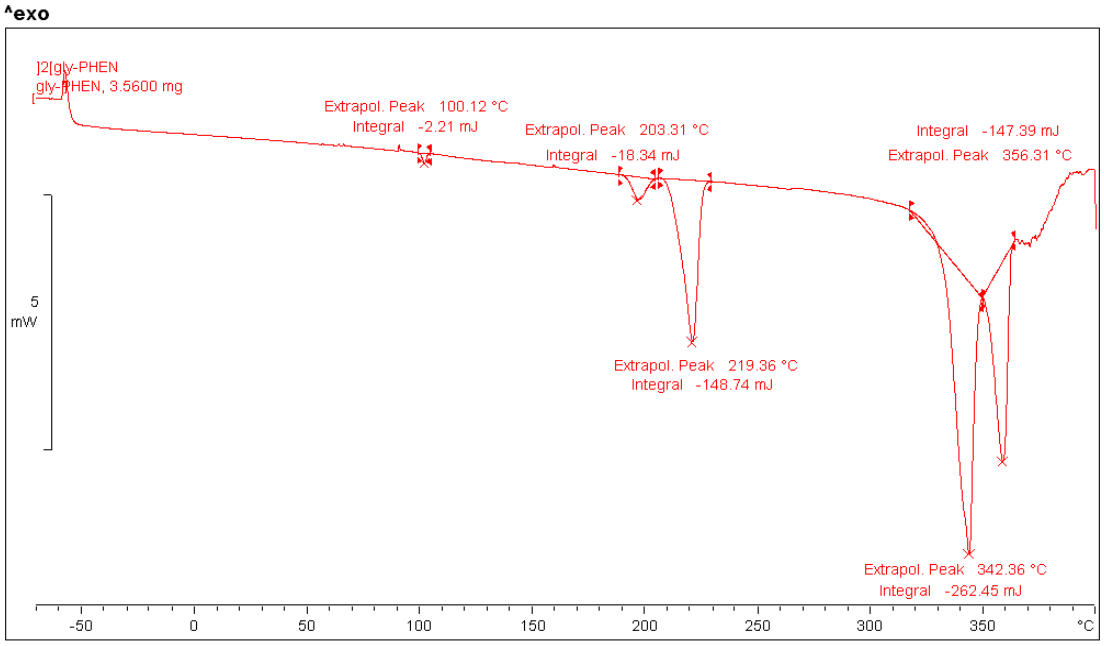


Figure A3.12: DSC curves of heat flow (mW) vs. temperature (^{o}C) for gly-PHEN.

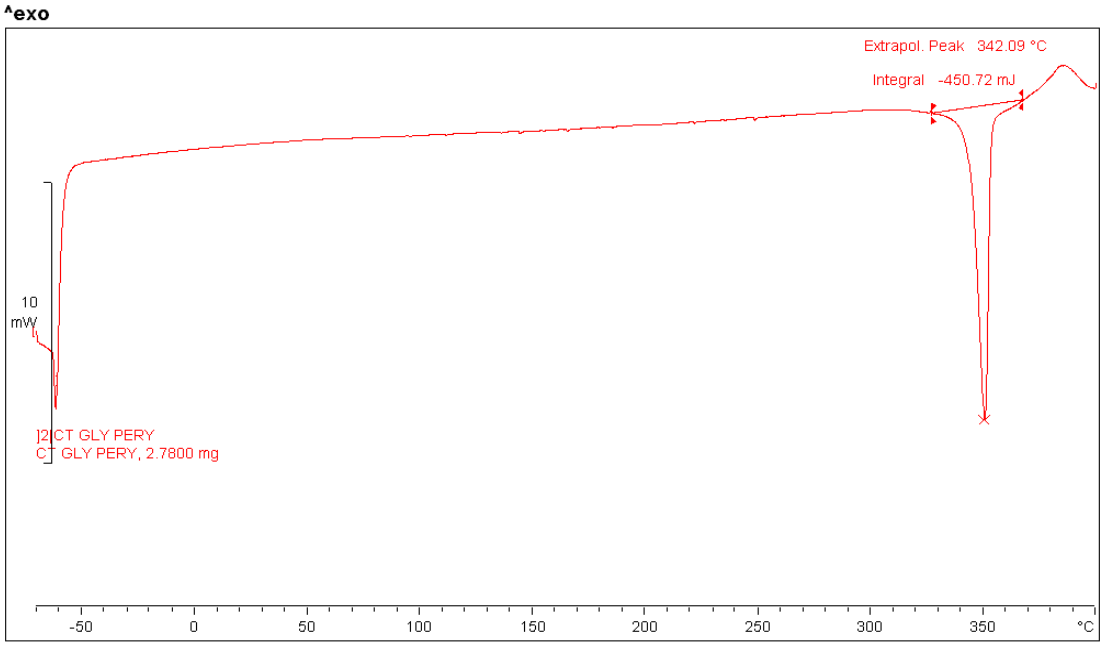


Figure A3.13: DSC curves of heat flow (mW) vs. temperature (^{o}C) for gly-PERY.

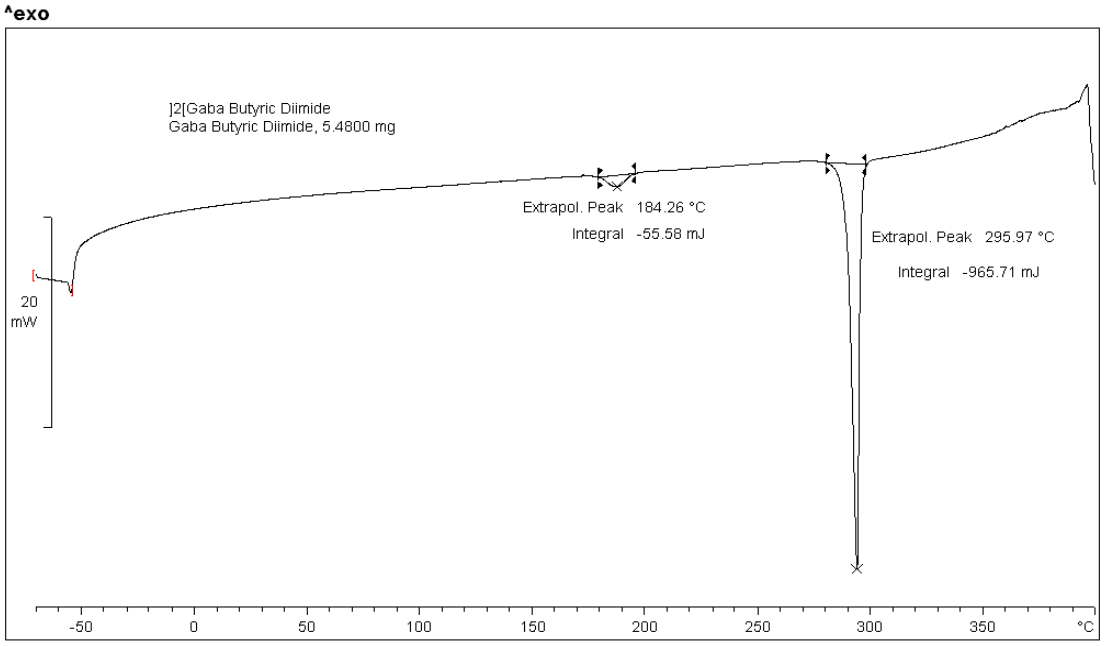


Figure A3.14: DSC curves of heat flow (mW) vs. temperature (^{o}C) for but-L.

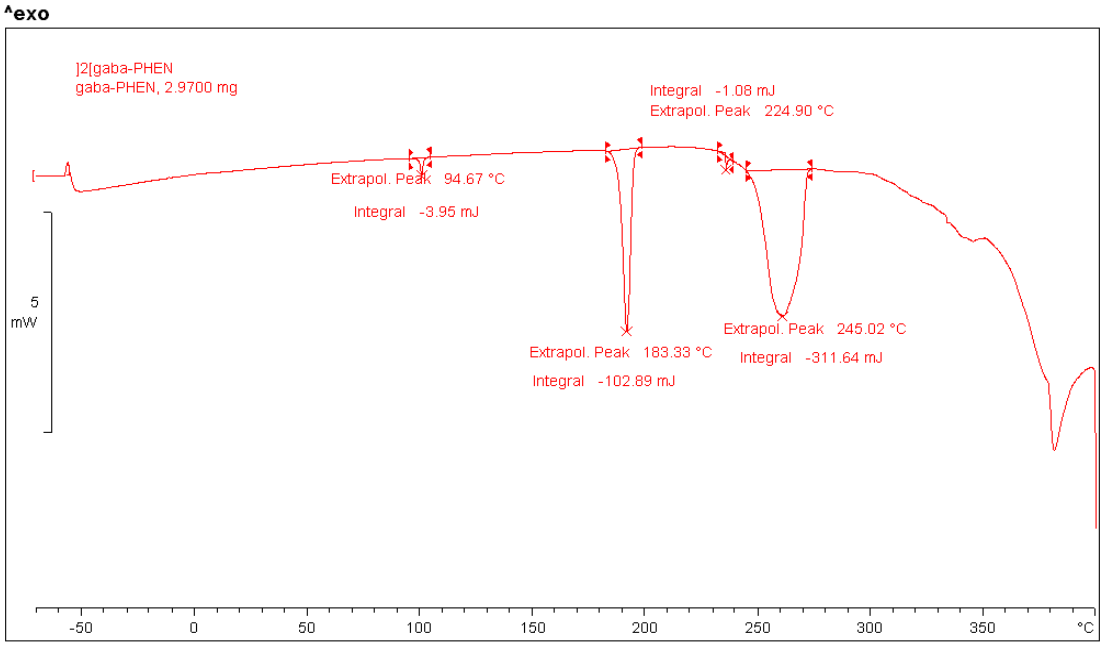


Figure A3.15: DSC curves of heat flow (mW) vs. temperature (^{o}C) for but-PHEN.

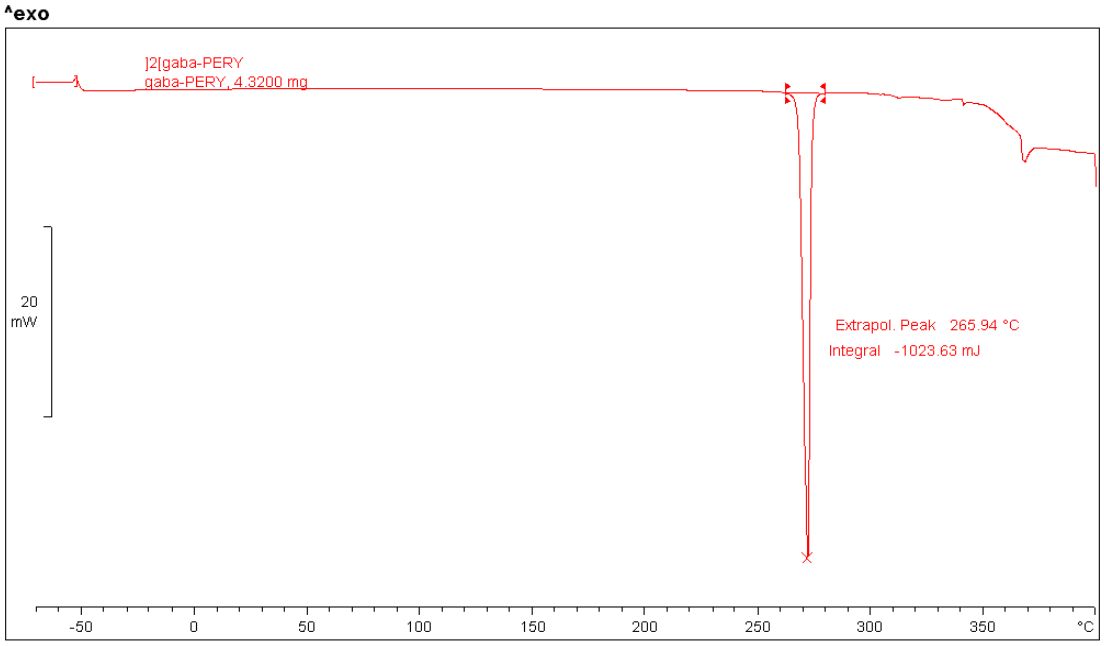


Figure A3.16: DSC curves of heat flow (mW) vs. temperature (^{o}C) for but-PERY.

Table A3.1: Calculated energies observed for DSC.

Complexes	Integral (mJ)	Mass (mg)	Molar mass (g/mol)	Moles (x 10^{-5} mol)	Enthalpy (kJ/mol)
gly-L	-413.52	4.34	322.22	1.35	-30.6
	-99.77				-7.39
gly-NAP	-906.81	5.13	460.39	1.11	-81.7
	-793.24				-71.5
gly-ANT	-1.60	1.56	574.53	0.272	-0.588
	-17.63				-6.48
	-107.15				-39.4
	-38.15				-14.0
	-16.85				-6.19
	-28.66				-10.5
	-95.07				-35.0
gly-PHEN	-2.21	3.56	510.44	0.697	-0.317
	-18.34				-2.63
	-148.74				-21.3
	-262.45				-37.7
	-147.39				-21.1
gly-PERY	-450.72	2.78	584.52	0.476	-94.7
but-L	-55.58	5.48	388.33	1.41	-3.94
	-965.71				-68.5
but-PHEN	-3.95	2.97	566.47	0.524	-0.754
	-102.89				-19.6
	-1.08				-0.206
	-311.64				-59.5
but-PERY	-1023.63	4.32	640.62	0.674	-152

Enthalpy = [(Integral (mJ) / Moles (x 10^{-5} mol)]) / 1000
= kJ/mol
Negative values indicate an exothermic reaction.

Appendix: A4 - Spectral Data

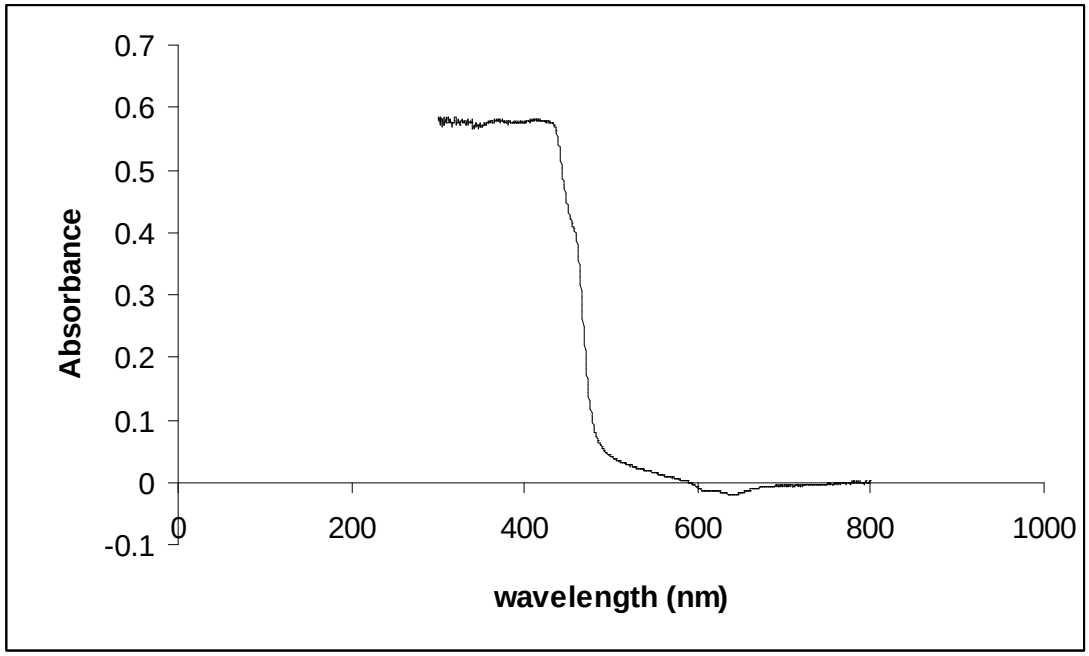


Figure A4.1: Solid state UV-Vis spectra for gly-NAP.

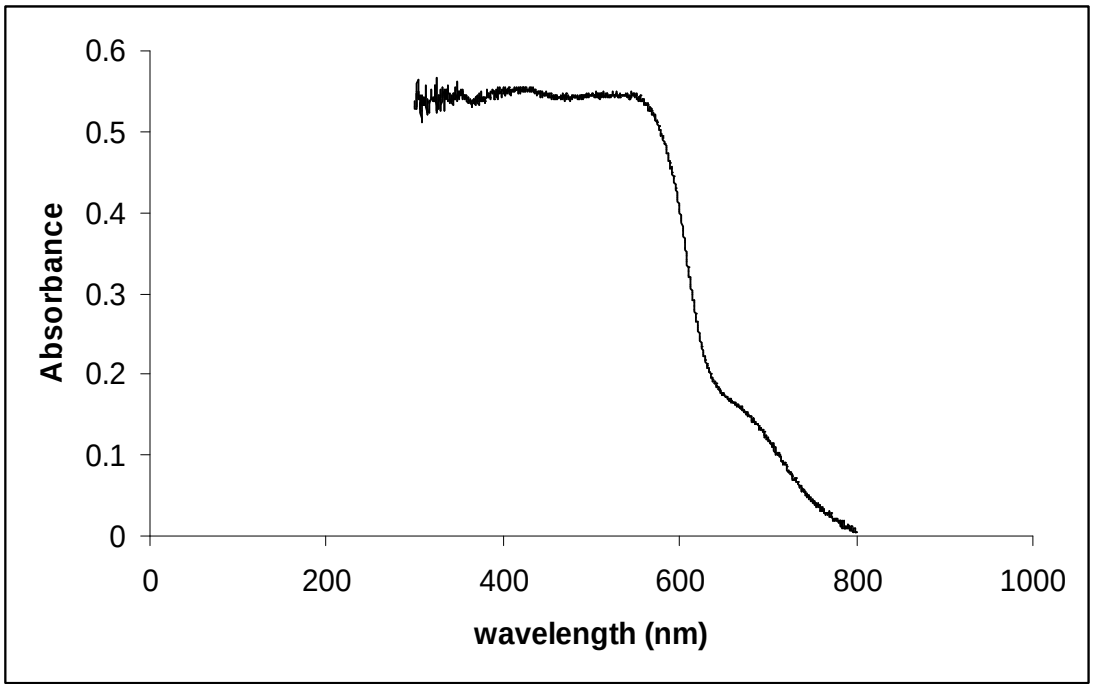


Figure A4.2: Solid state UV-Vis spectra for gly-ANT.

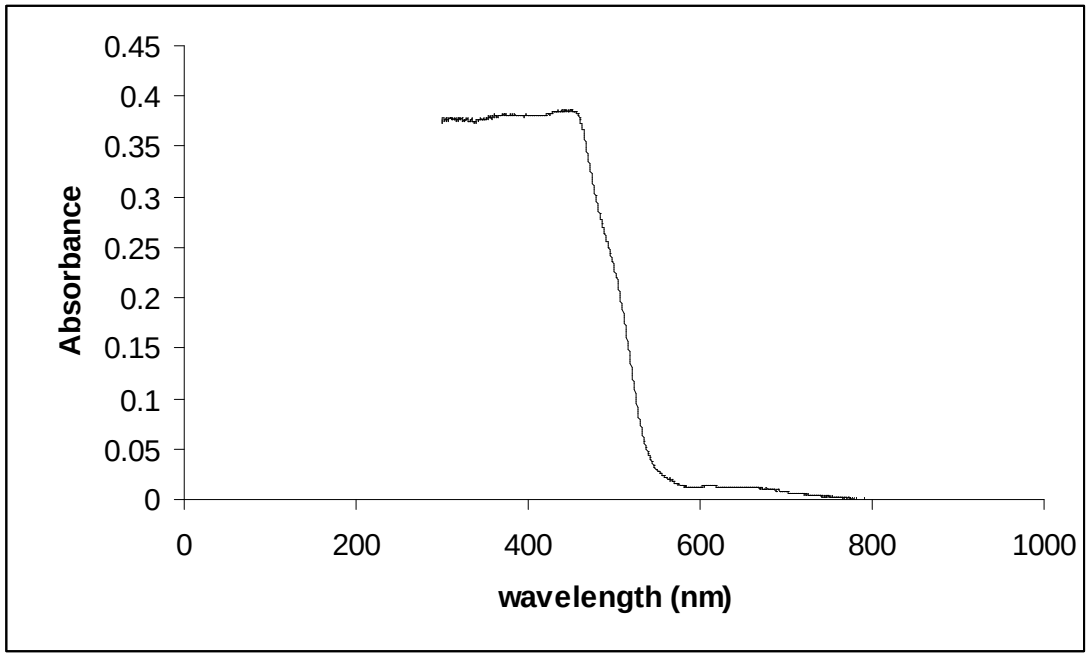


Figure A4.3: Solid state UV-Vis spectra for gly-PHEN.

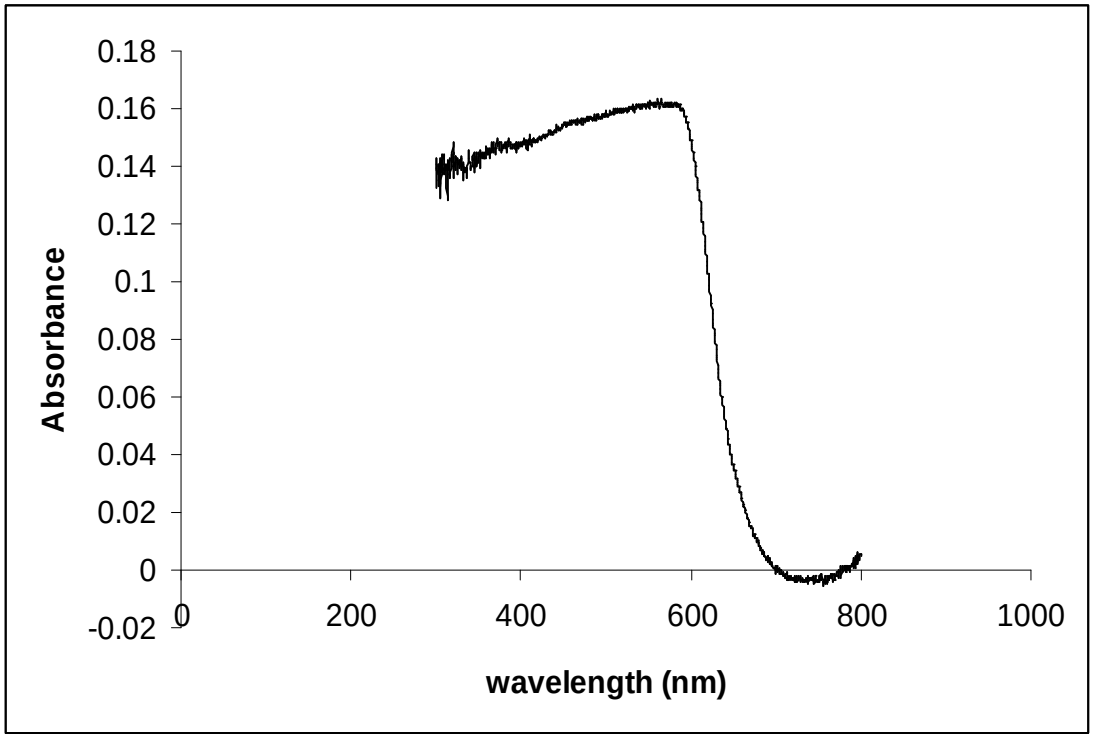


Figure A4.4: Solid state UV-Vis spectra for gly-PERY.

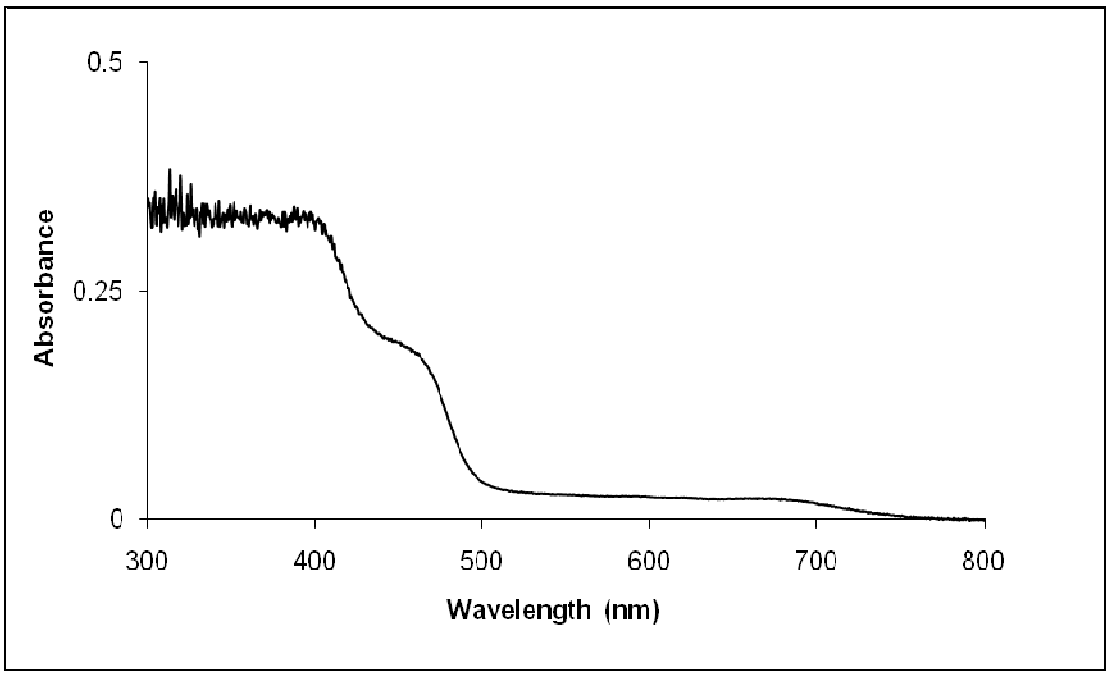


Figure A4.5: Solid state UV-Vis spectra for but-PHEN.

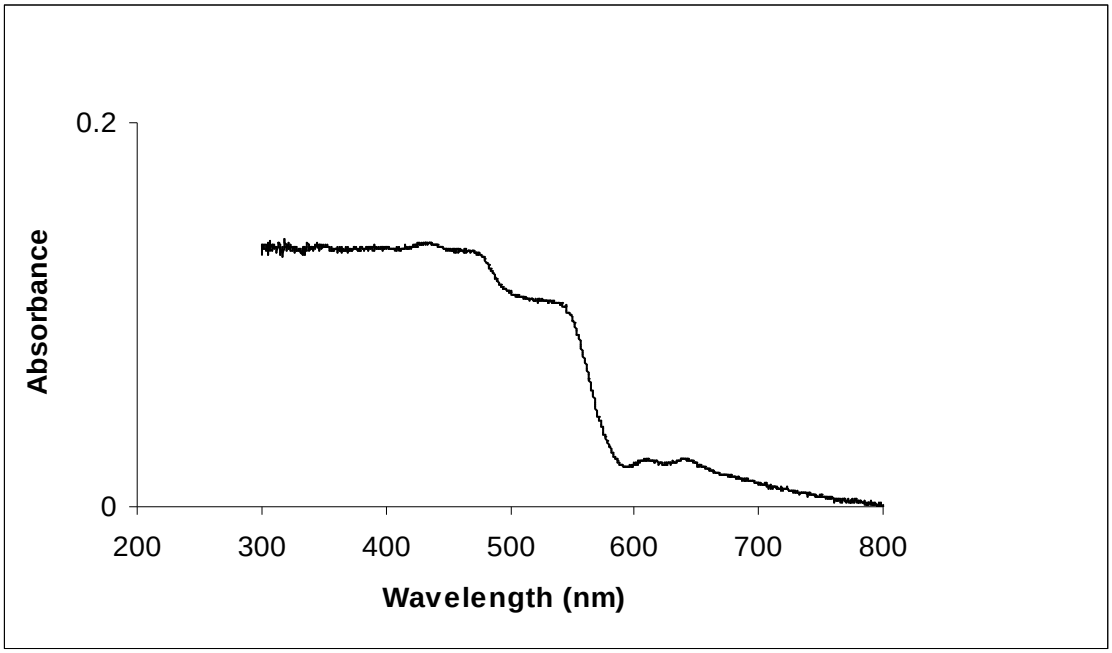


Figure A4.6: Solid state UV-Vis spectra for but-PERY.

Table A4.1: Calculated energies associated with solid state transition bands.

Complexes	Transition band (λ, nm)	Energy (kJ/mol)
gly-NAP	597	200
gly-ANT	800	149
gly-PHEN	584	205
gly-PERY	721	166
but-PHEN	534	224
	448	267
but-PERY	592	202
	499	240

Energy = hc/λ x N

Where h (Planck's constant) : $6.62606876 \times 10^{-34}$ J/s
c (Speed of light) : 2.99792458×10^{8} m/s
and N (Avogadro's no.) : $6.02214199 \times 10^{23}$/mol

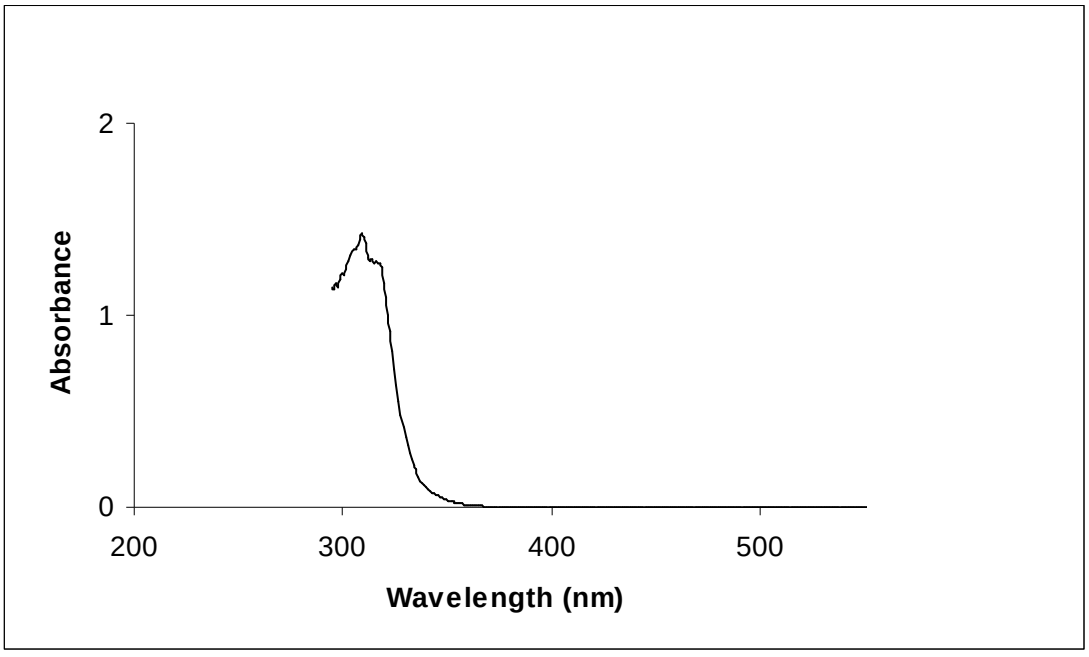


Figure A4.7: Liquid state UV-Vis spectra for gly-NAP.

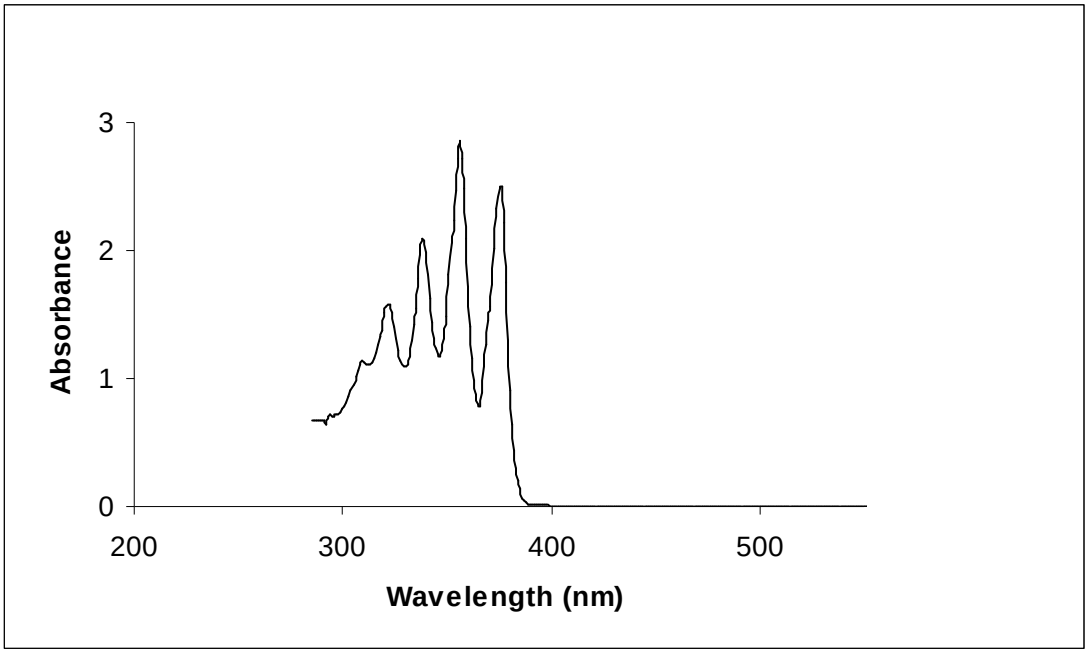


Figure A4.8: Liquid state UV-Vis spectra for gly-ANT.

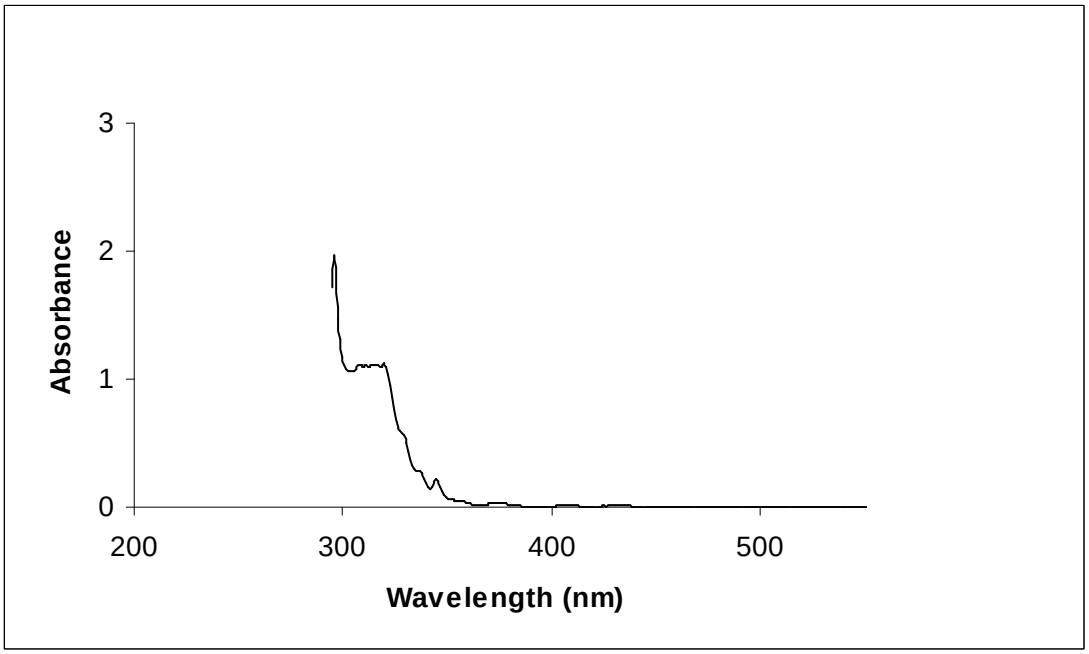


Figure A4.9: Liquid state UV-Vis spectra for gly-PHEN.

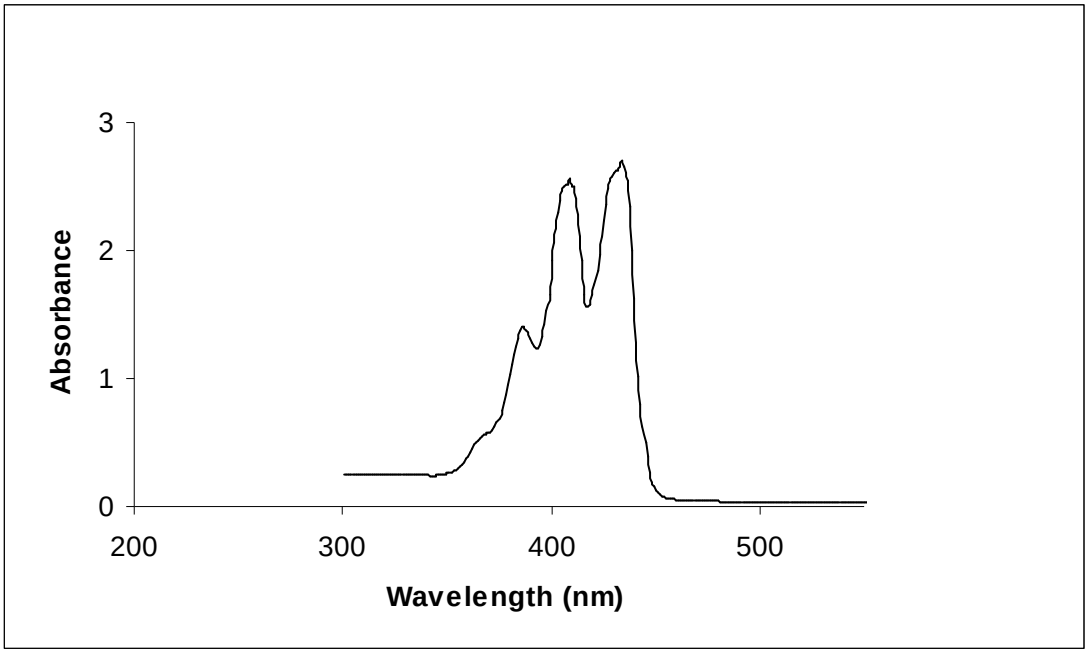


Figure A4.10: Liquid state UV-Vis spectra for gly-PERY.

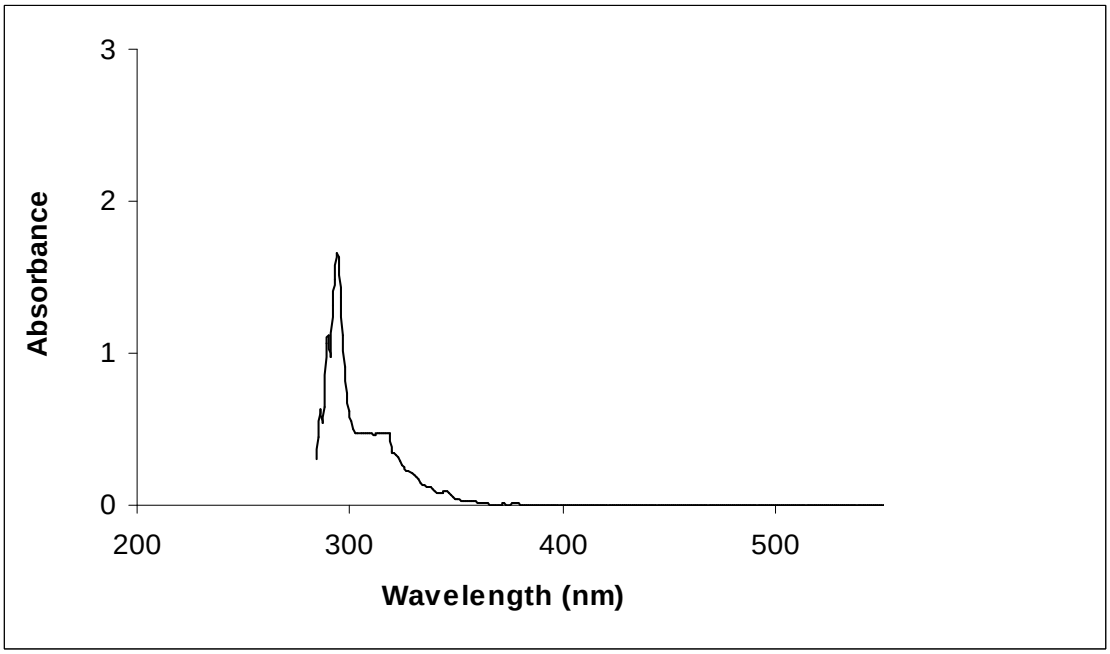


Figure A4.11: Liquid state UV-Vis spectra for but-PHEN.

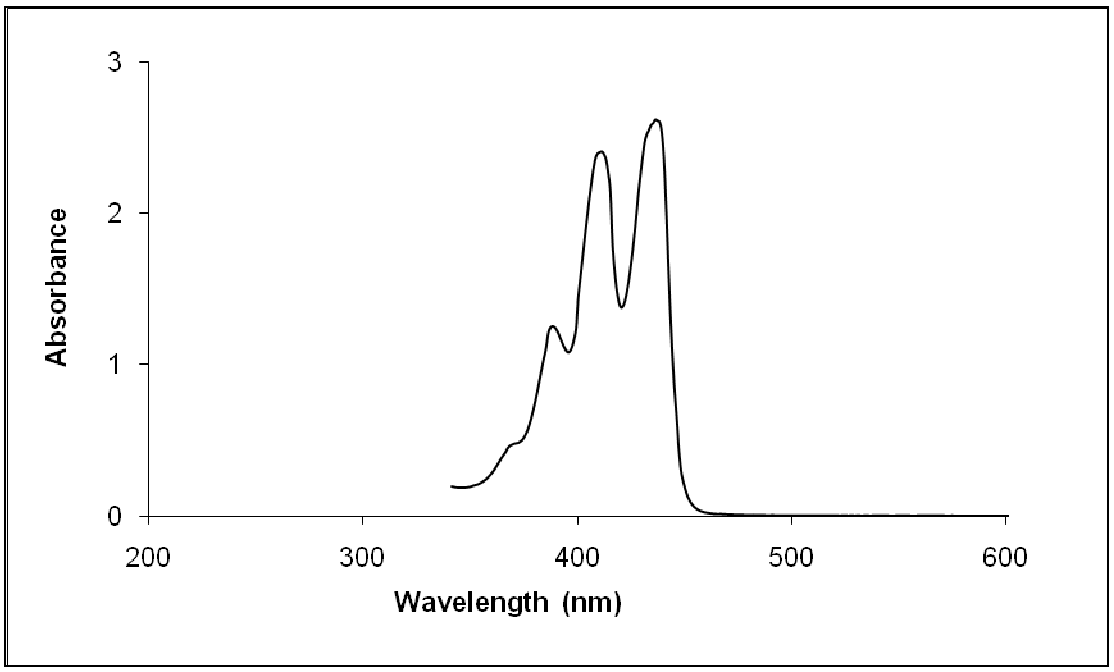


Figure A4.12: Liquid state UV-Vis spectra for but-PERY.

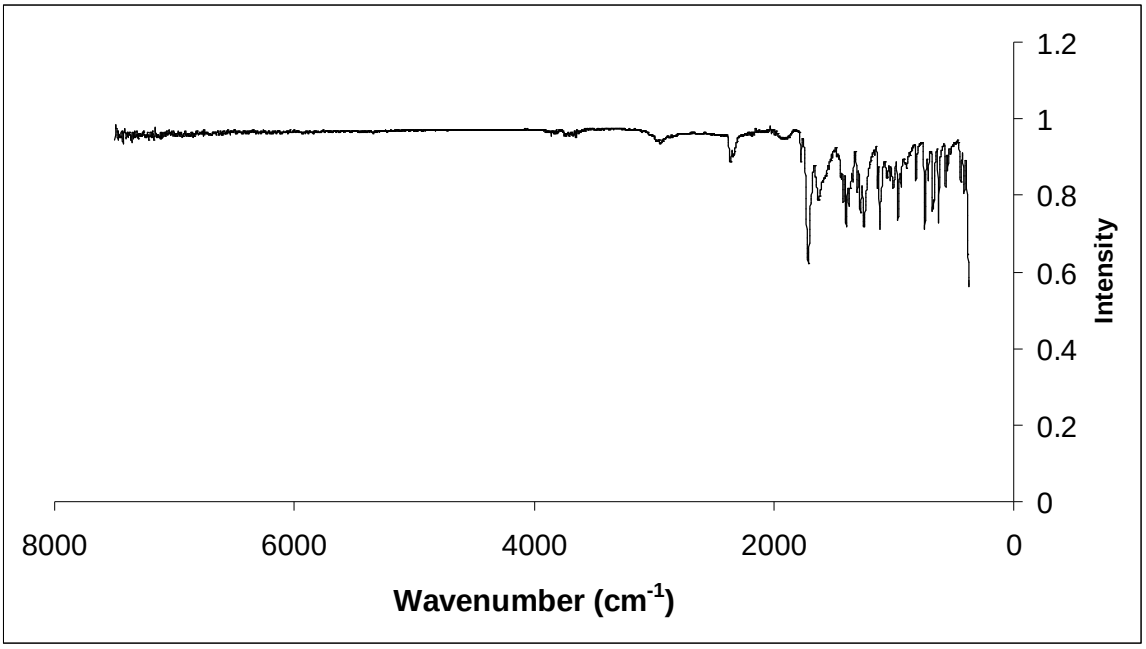


Figure A4.13: IR spectrum for gly-L.

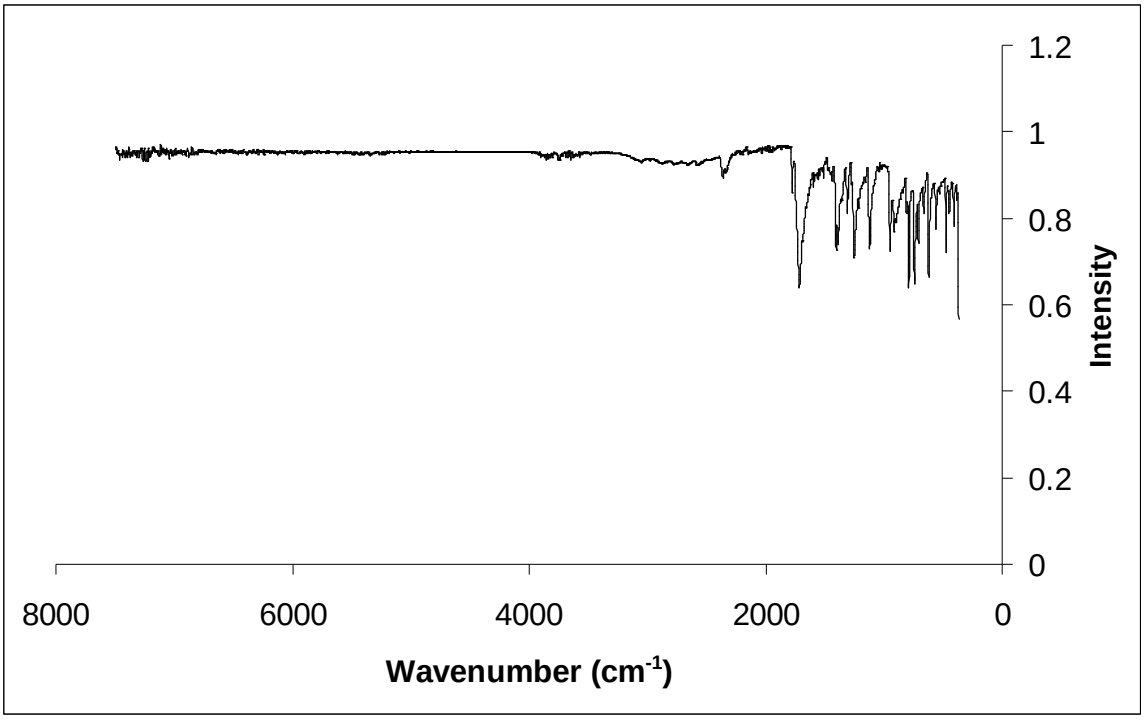


Figure A4.14: IR spectrum for gly-NAP.

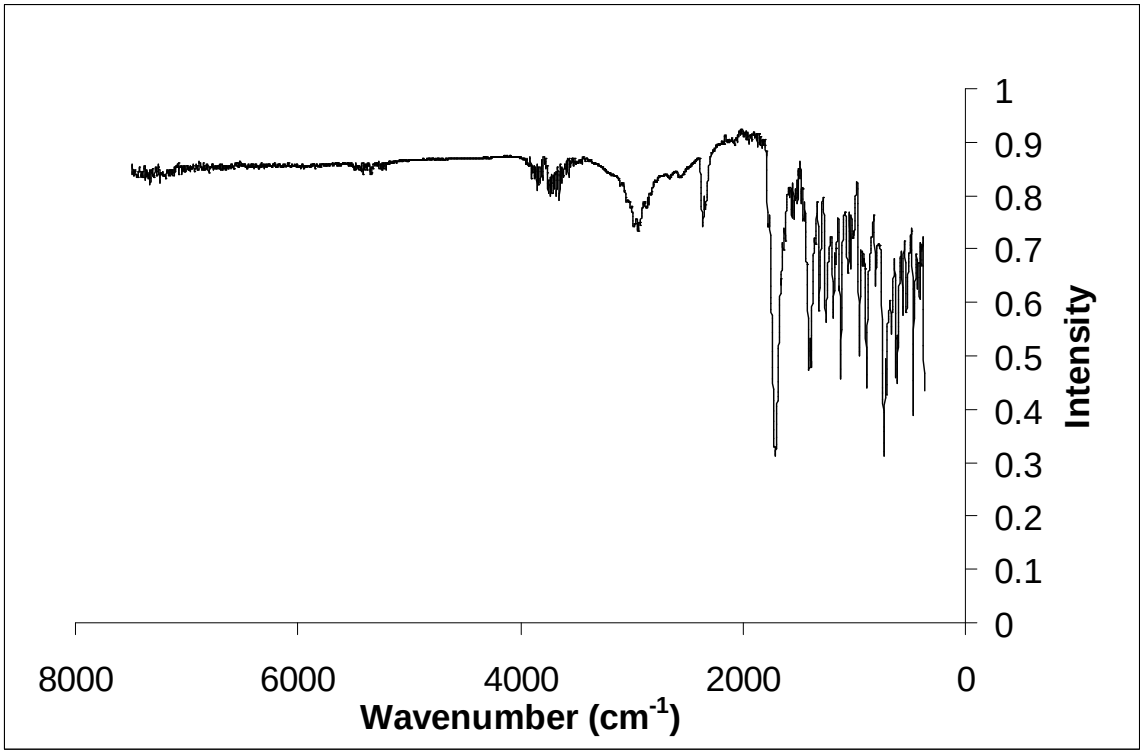


Figure A4.15: IR spectrum for gly-ANT.

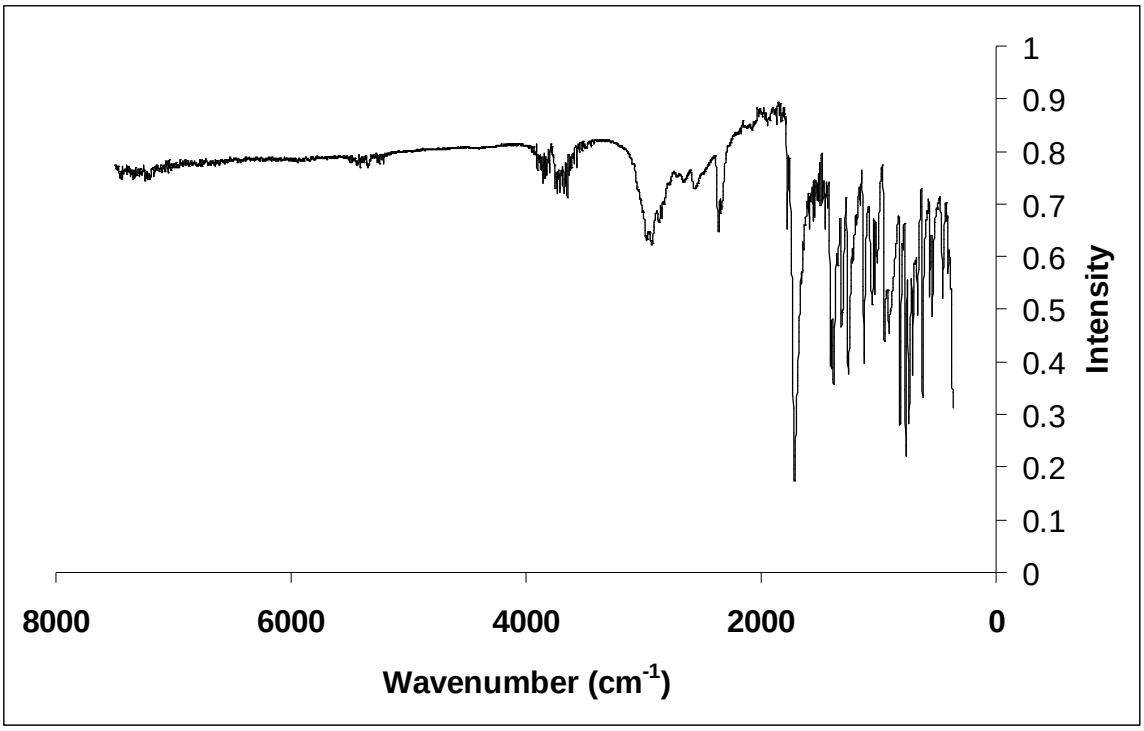


Figure A4.16: IR spectrum for gly-PHEN.

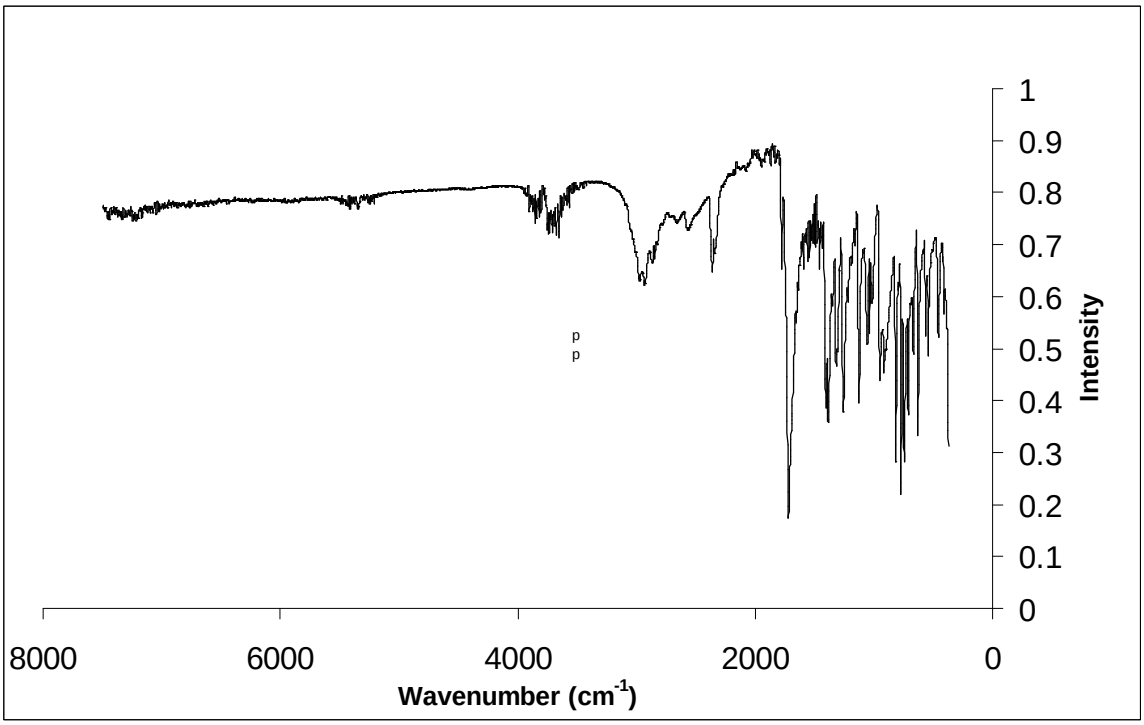


Figure A4.17: IR spectrum for gly-PERY.

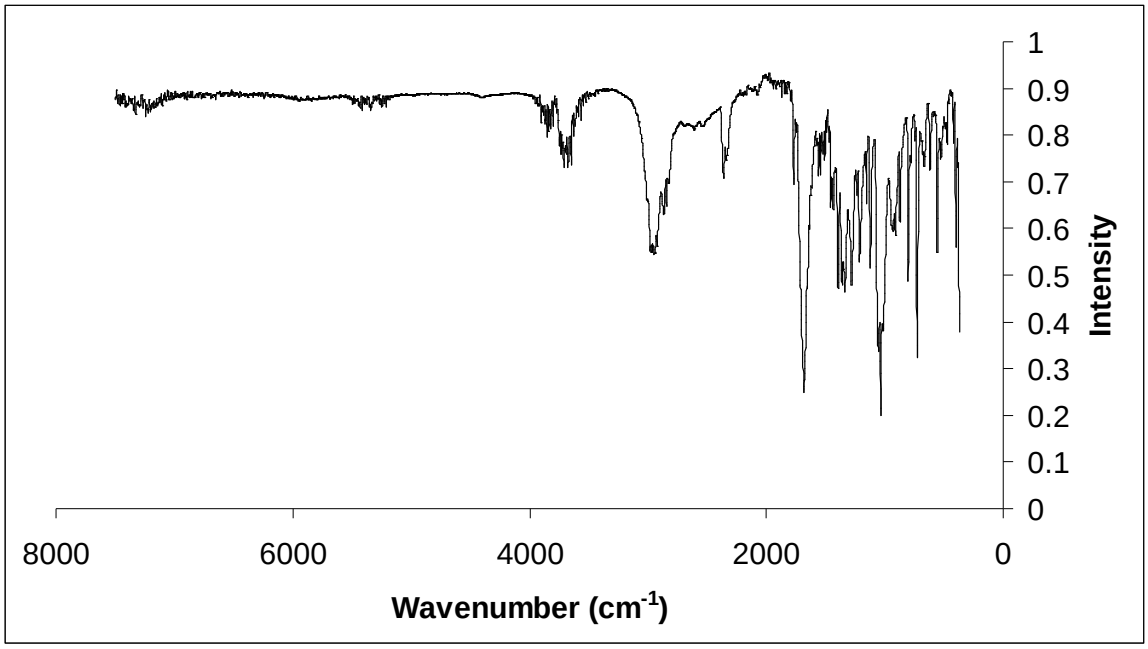


Figure A4.18: IR spectrum for but-L.

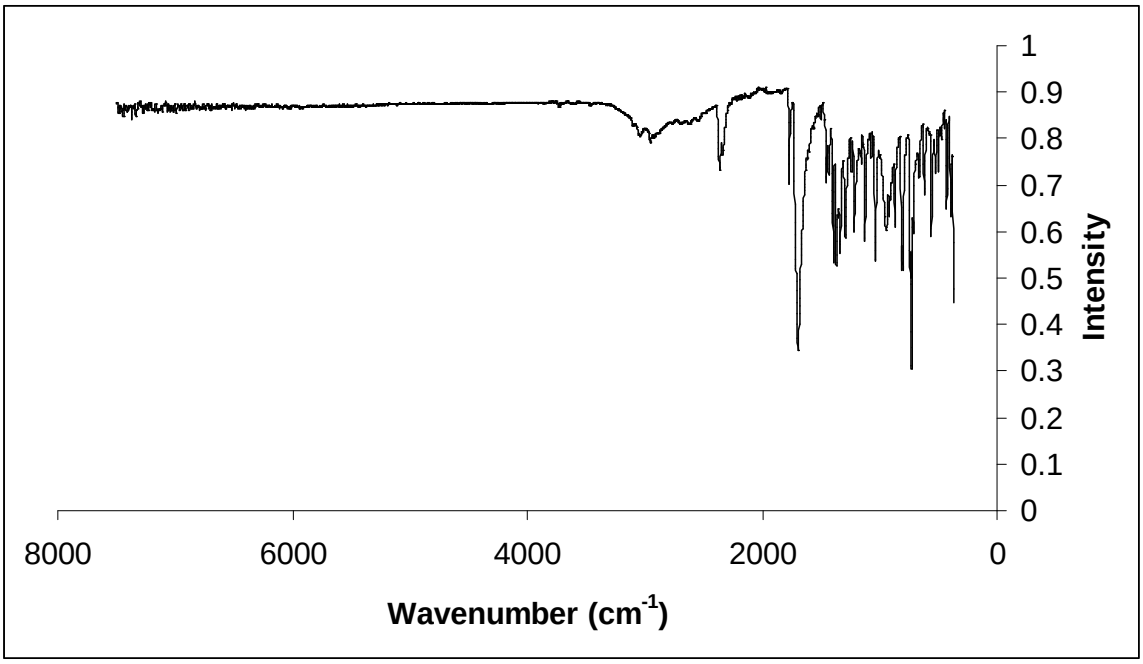


Figure A4.19: IR spectrum for but-PHEN.

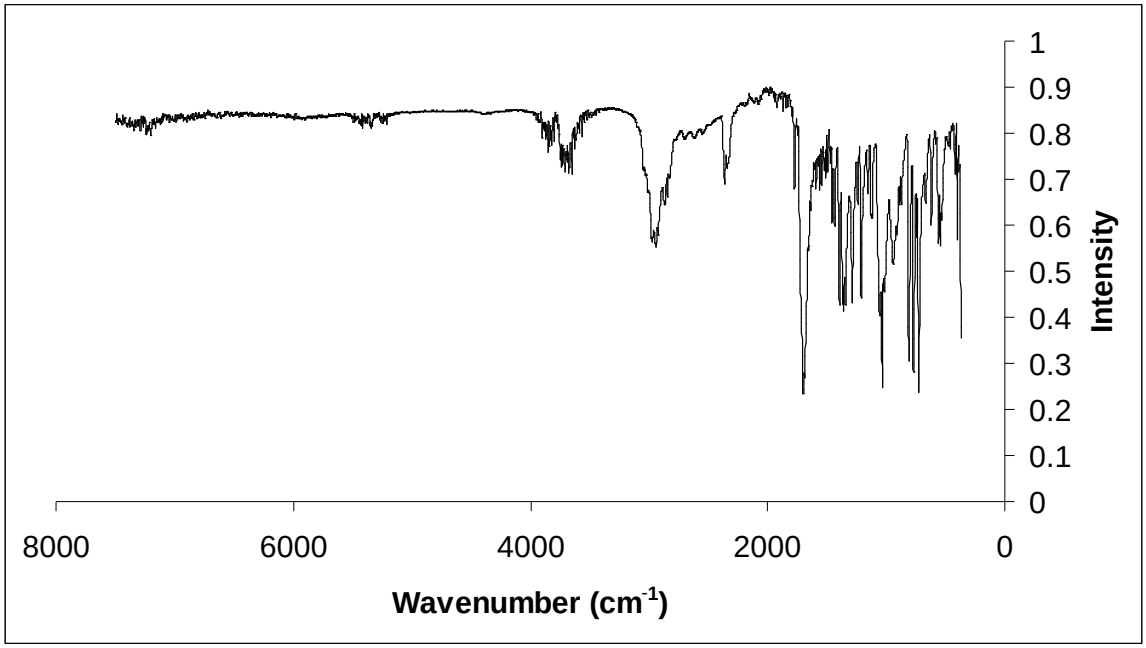


Figure A4.20: IR spectrum for but-PERY.

Appendix: A5 – Submitted cif.files