Electronic Supplementary Material (ESI) for CrystEngComm

Supplementary Information

Evaluation of the Role of Disordered Organic Fluorine in Crystal Packing: Insights from halogen substituted Benzanilides.

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TABLE S1: Dihedral angles between least squares Plane 1, Plane 2 and Plane 3

(Plane 1 = C1/C2/C3/C4/C5/C6; Plane 2 = O1/C1/N1; Plane 3 = C8/C9/C10/C11/C12/C13;)

	Plane 1-Plane 2/°	**Plane 1-Plane 3/°**	**Plane 2-Plane 3/°**
2FA-2IB	64.4(1)	67.1(1)	47.9(2)
3FA-2ClB	53.2(1)	36.2(1)	17.0(1)
3FA-2BrB	54.8(1)	83.6(1)	29.0(1)
3FA-2IB	56.7(1)	84.9(1)	28.6(1)
3FA-3BrB	33.4(1)	71.5((1)	38.9(1)
2FB-2ClA	32.1(1)	3.7(1)	32.1(1)
2FB-2BrA	34.2(1)	4.8(2)	34.4(1)
2FB-2IA	38.1(1)	6.0(1)	38.3(2)
3FB-4ClA	31.5(2)	67.0(1)	36.6(2)
3FB-4BrA	31.1(1)	67.3(1)	36.9(1)

TABLE S2: Crystallization solvents, size and morphology/color of the crystals

	Crystallization from Solvents	**Size of Crystal (Data Collected)**	**Morphology/Color of crystals**
2FA-2IB	Ethyl acetate/Hexane (v/v- 1:1)	0.22×0.18×0.13	Block/colorless
3FA-2ClB	Ethyl acetate/Hexane (v/v- 1:1)	0.30×0.19×0.11	Plate/colorless
3FA-2BrB	Ethyl acetate/Acetonitrile(v/v- 1:1)	0.24×0.23×0.16	Plate/colorless
3FA-2IB	Dichloromethane/Hexane(v/v- 1:1)	0.20×0.14×0.10	Block/colorless
3FA-3BrB	Ethyl acetate/Hexane (v/v- 1:1)	0.25×0.19×0.14	Plate/colorless
2FB-2ClA	Ethyl acetate/Acetonitrile(v/v- 1:1)	0.30×0.28×0.19	Block/colorless
2FB-2BrA	Ethyl acetate/Hexane (v/v- 1:1)	0.30×0.24×0.11	Plate/colorless
2FB-2IA	Ethyl acetate/Acetonitrile(v/v- 1:1)	0.30×0.28×0.22	Block/colorless
3FB-4ClA	Dichloromethane/Hexane(v/v- 1:1)	0.28×0.19×0.10	Plate/colorless
3FB-4BrA	Ethyl acetate/Hexane (v/v- 1:1)	0.29×0.17×0.09	Plate/colorless

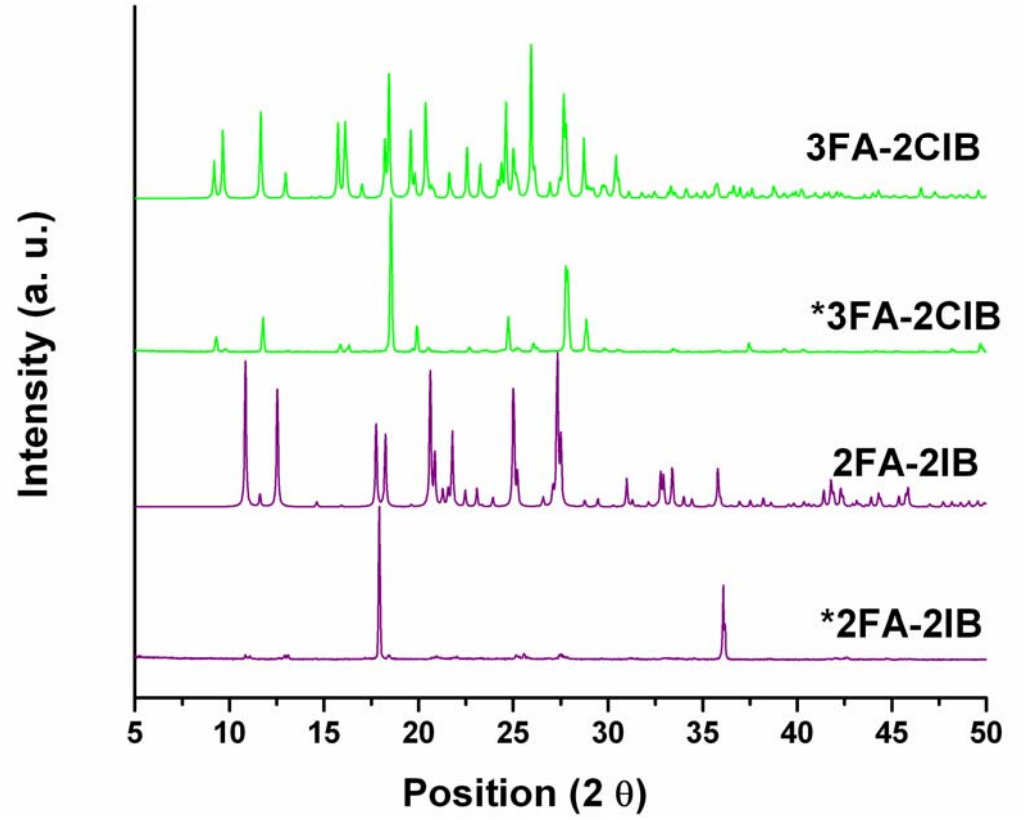
TABLE S3: List for the disordered structures exhibiting disorder either at both *ortho* sites *or meta* sites by halogen atom, CSDCODE and the atom in bracket indicates that disorder is associated with the corresponding halogen atom.

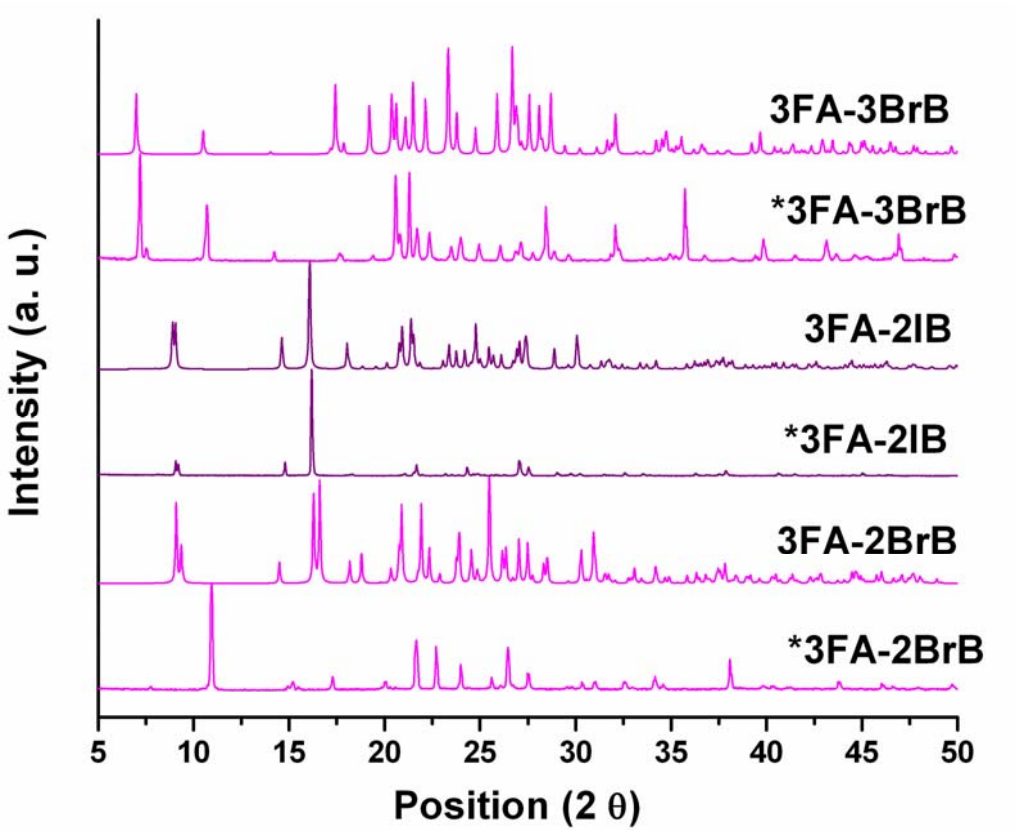
2-F Substituted				
ADEYIS(H)	AKIWUM(H)	AWITEF(H)	*BIMCAC(H)*	*BOPNOK(H)*
BOWTUD(H)	*CAYVII(H)*	*CEJTER(H)*	CIQLET(H)	COCCIG(H)
COZDOK(H)	CUBNIX(H)	DAJGIE(H)	EBETAH(H)	FABTIM(H)
FAFWIS(H)	FAFWIS(H)	FAWJET(H)	FAWJIX(H)	*FLUBIP01(H)*
FLUBIP02(H)	FOPCET(H)	FOCOJ(H)	*GIJLUH(H)*	GIPKEV(H)
HAYWAG(H)	HAZHIA(H)	HOQRUA(H)	HORGIE(H)	HUPPEN(H)
HUPPIR(H)	*HUPVOE(H)*	*HUPVUK(H)*	IDAHOL(H)	IYIYOE(H)
KASPAV(H)	*KUCGOF(H)*	KUTJAL(H)	LAHPER(H)	LAWDAP(H)
LIJXAE(H)	*LODFUF(H)*	LURMUG(H)	LUZJUM(H)	MEBJEJ(H)
MEKMUL(H)	*MIHPID(H)*	MITHEC(H)	MOKWIT(H)	MOSPUG(H)
NAXCUL(H)	NAYWOA(H)	NEFSOH(H)	NIHBAH(H)	NIHBAH01(H)
NUJWUL(H)	NUXKAS(H)	OCIQEX(H)	ODIXUV(H)	PEQPUX(H)
POMVIX(H)	QADLUD(H)	QAJVII(H)	QAJZAE(H)	QAMWEH(H)
QIGFUH(H)	*QOQVOI(H)*	*QUPLAP(H)*	REZZAX(H)	SADSUN(H)
SAZKOU(H)	SOLSUI(H)	SUZKII(H)	*TATLUW(H)*	*TECMAQ(H)*
TESQEO(H)	TESQEO01(H)	TIDRAA(H)	VEGGIX(H)	WAVRUH(H)
WOBCAS(H)	WOBDAT(H)	WUFXAX(H)	WUFXEB(H)	*WUTXEP(H)*
WUTXUF(H)	XEZHIU(H)	XIQZAZ(H)	XIZBUE(H)	*XOQTUT(H)*
XOQVAB(H)	XOZMAB(H)	**XUDREU(H)**	YOKLAM(H)	YOVNIH(H)
ZEHDIZ(H)	*ZENRAL(H)*			
		3-F Substituted		
ADEYIS(H)	BICYES(H)	*BIMCAC(H)*	*BOPNOK(H)*	CAYVII(H)
CEJTER(H)	CIYXAK(H)	CIYXAK01(H)	COCCIG(H)	DEHXUK(H)
DEHYAR(H)	DICSIS(H)	DOKXOR(H)	DUZLIU(H)	FABTIM(H)
FAFWIS01(H)	*FLUBIP02(H)*	FOVCOJ(H)	*GIJLUH(H)*	HOLJAU(H)
HORMUX(H)	HUPPEN(H)	HUPPIR(H)	*HUPPVOE(H)*	*HUPVUK(H)*
IDOWAA(H)	IHOWAE(H)	JEMSOK(H)	KALFIN(H)	*KUCGOF(H)*
KUDXUD(H)	KUDYAK(H)	KUTJAL(H)	KUYZOU(H)	LAHPER(H)
LIJXAE(H)	*LODFUF(H)*	LURMUG(H)	LUZJUM(H)	MEBJEJ(H)
MEKMUL(H)	*MIHPID(H)*	MOSPUG(H)	MUCJUQ(H)	MUYLOH(H)
NAXCUL(H)	NIHBAH(H)	NIHBAH01(H)	NOQVEW(H)	NULXAT(H)
NUXKAS(H)	ODIXUV(H)	PEQPUX(H)	PEVFIG(H)	PIYGEJ(H)
QAYRUE(H)	QENTIN(H)	*QIGFUH(H)*	*QOQVOIP(H)*	*QUPLAP(H)*
RIRZEY(H)	RUXSAE(H)	SACLOZ(H)	*SAZKOU(H)*	SOBBER(H)
TATLUW(H)	*TECMAQ(H)*	UMUQUO(H)	VUJFEM(H)	VUQGUK(H)
WADHIU(H)	WOBCAS(H)	WONMIK(H)	*WUTXEP(H)*	*WUTXUF(H)*
XIFVUE(H)	*XOQTON*(H)	*XOQTUT*(H)	*XOQVAB(H)*	YIQDOS(H)
YUNYUB(H)	*ZENRAL(H)*			

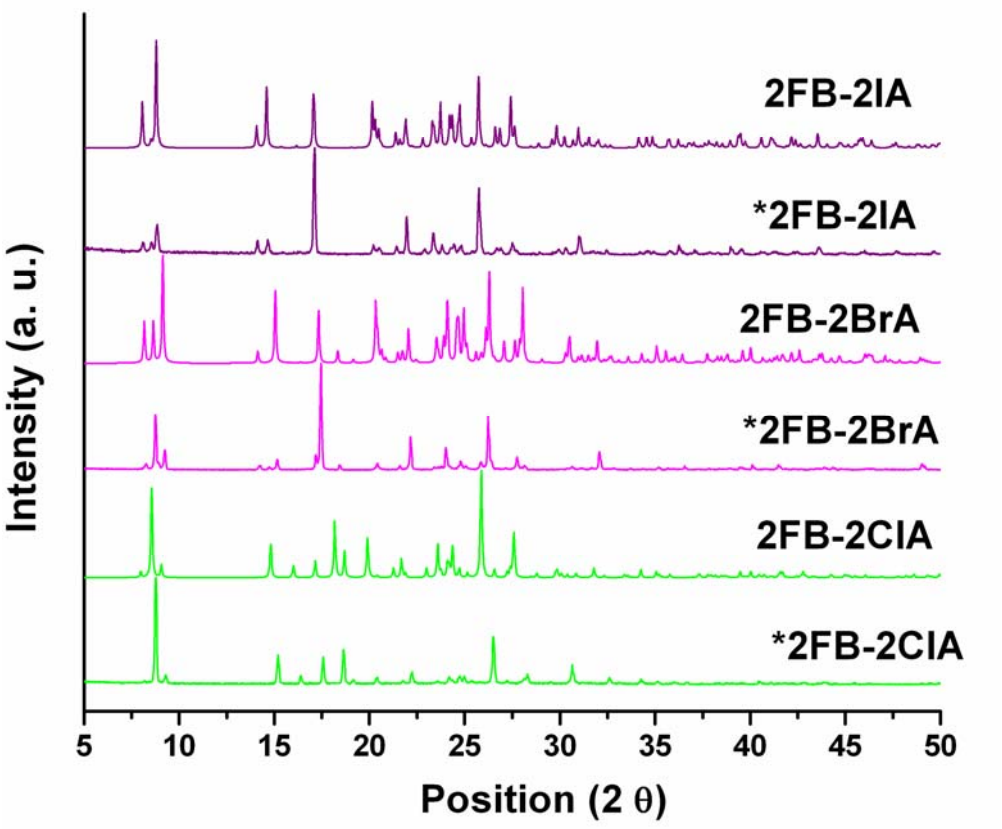
TABLE S2: Contd…

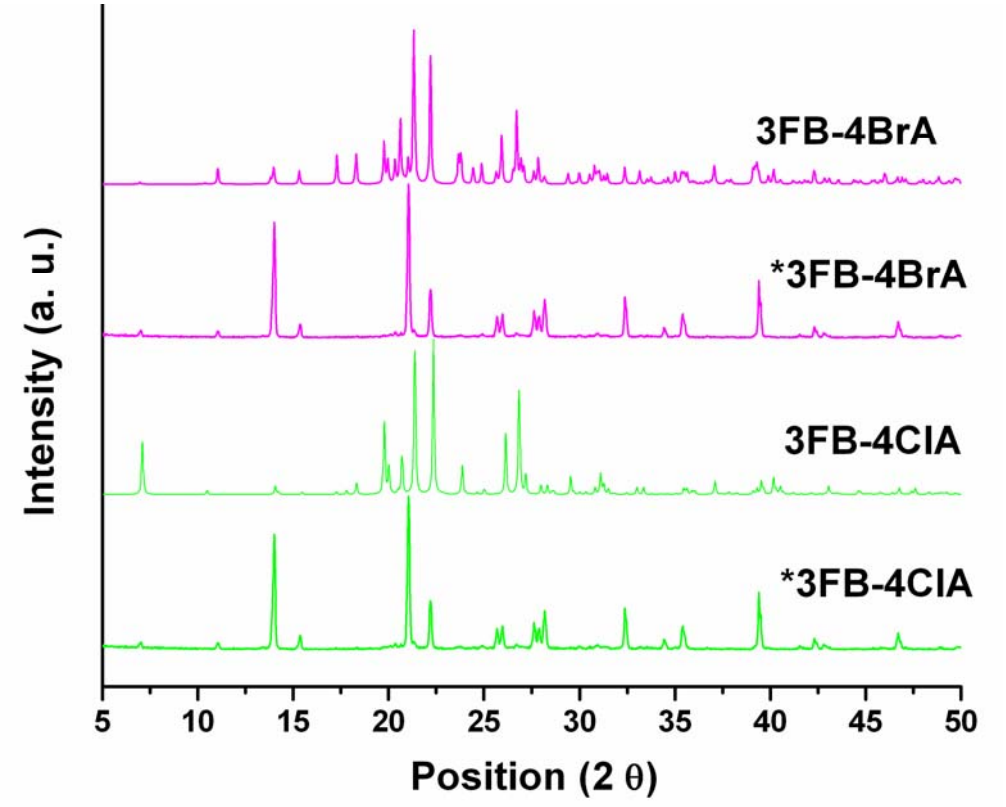
		2-Cl Substituted		
DADZEO(H)	CUBNIX(CF_3)	*DBTCBEO01(Br)*	*FOMLOJ(Br)*	IHATIU(Me)
DAQMUD(H)	JOCMIY(NO_2)	KEBWUK(Me)	KEBWUK01(Me)	LATWIM(Me)
DUNBAQ(H)	NULVOG(Me)	RAZZO1(NO_2)	*SEDDUA(Br)*	*TUSQAZ(Br)*
EYIZOB(H)	XEZFOY(Me)	XIKKOS(NO_2)		
IREKUL(H)	MIGBEG(H)	*NERCOD(H)*	*SUTTUX(H)*	WAQVAL(H)
		3-Cl Substituted		
DADZEO(H)	*DBTCBEO01(Br)*	DUNDOG(Br)	FADQEH(H)	*FOMLOJ(Br)*
GUVXAX(Cl)	KAQJOB(NO_2)	*NERCOD(H)*	QAXFEB(H)	*SEDDUA(Br)*
SUTTUX(H)	*TUSQAZ(Br)*	UFUCIH(H)	VASLUX(H)	VUWBUL(H)
		2-Br Substituted		
Only one hit for disorder at *ortho site* with Hydrogen atom (**POZDIS**), whereas few more numbers other heavy atoms or other function groups (listed below) besides disorder mainly in other parts of the molecule				
ABEPET(Me)	*AJISAO(I)*	EBOBEC(OMe)	*EBOBIG(OMe)*	*FOMLOJ(Cl)*
PEPHUO(NO_2)	RIRXEW(OMe)	*SEDDUA(Cl)*	TUSQAZ(Cl)	XIKLUZ(NO_2)
		3-Br Substituted		
ABEPET(Me)	*AJISAO(I)*	*EBOBIG(OMe)*	*FOMLOJ(Cl)*	*SEDDUA(Cl)*
		2-I substituted		
There is no structure having both *ortho* sites disorder of Iodine atom with hydrogen atom, however few structures shows disorder at both *ortho* sites with other heavy atoms or function groups (listed below)				
ACIGAU (Methyl)	*AJISAO(Bromine)*	*OMOKQ(NO_2)*	*UCEQEZ(Cl)*	*UCEQOZ(Br)*
		3-I substituted		
There is no structure having both meta site disorder of Iodine atom with hydrogen atom, however few structures shows disorder at both *meta* sites with other heavy atoms or function groups (listed below) (Which comes under same hits are written as italics)				
ACIGAU (Methyl)	*AJISAO(Bromine)*	*OMOKQ(NO_2)*	*UCEQEZ(Cl)*	*UCEQOZ(Br)*

Powder X-ray Data for the polycrystalline samples* are compared with simulated Powder X-ray Pattern.

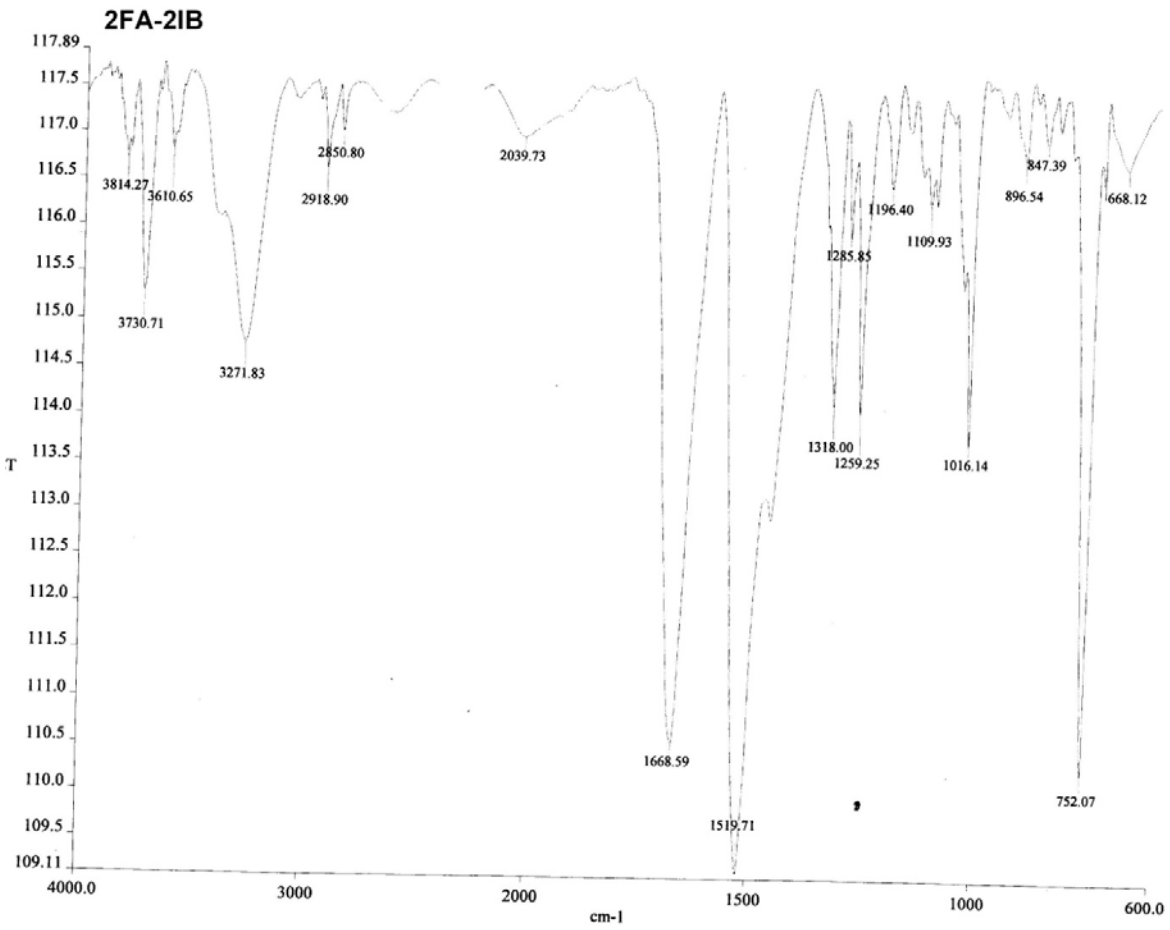






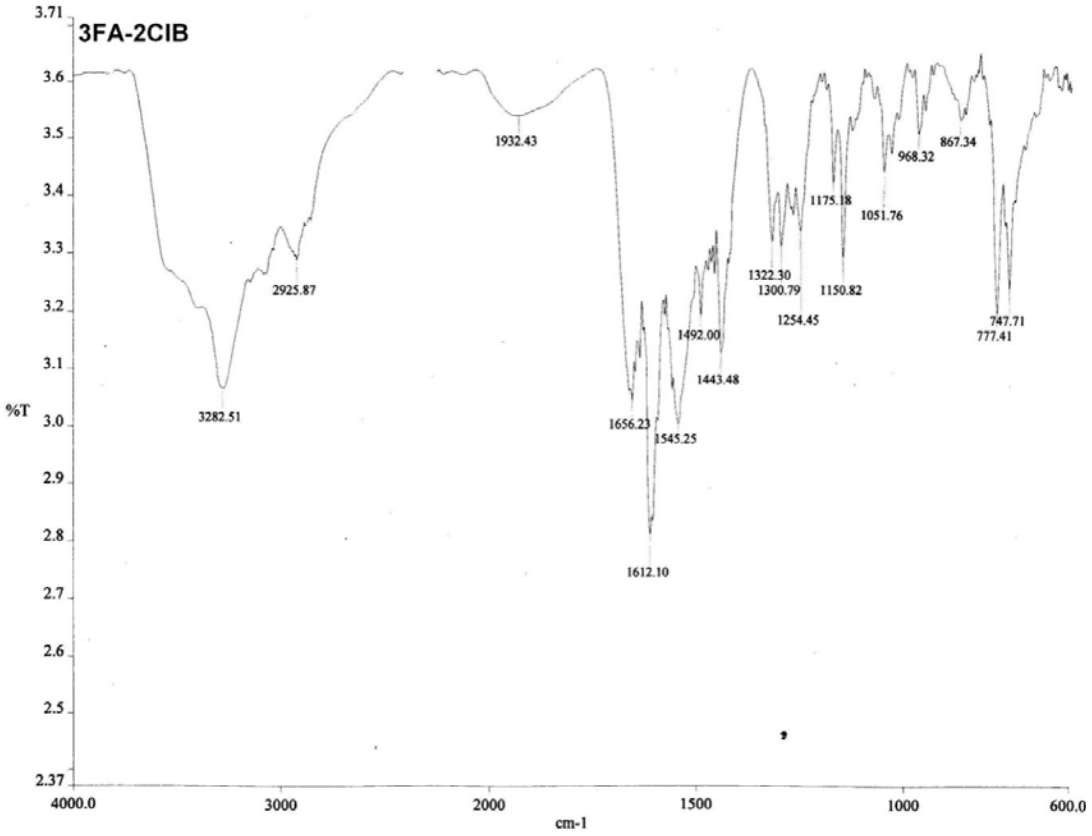


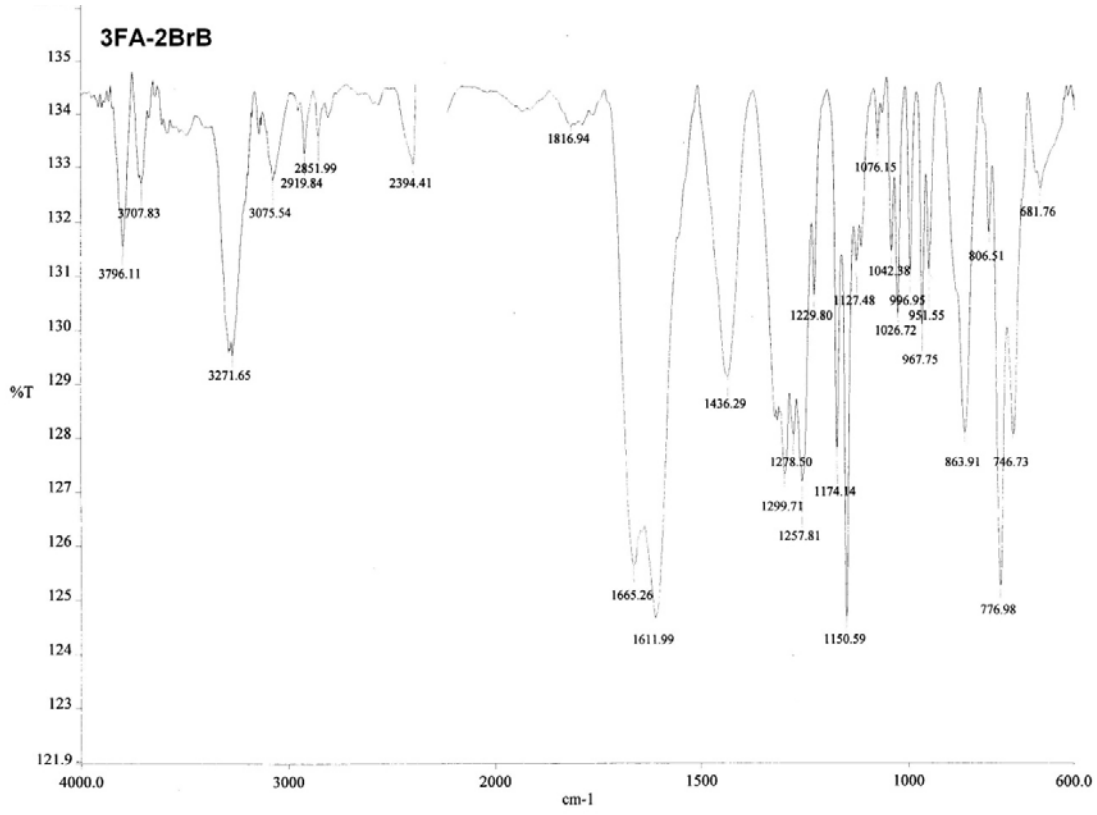
IR DATA are listed as follows:

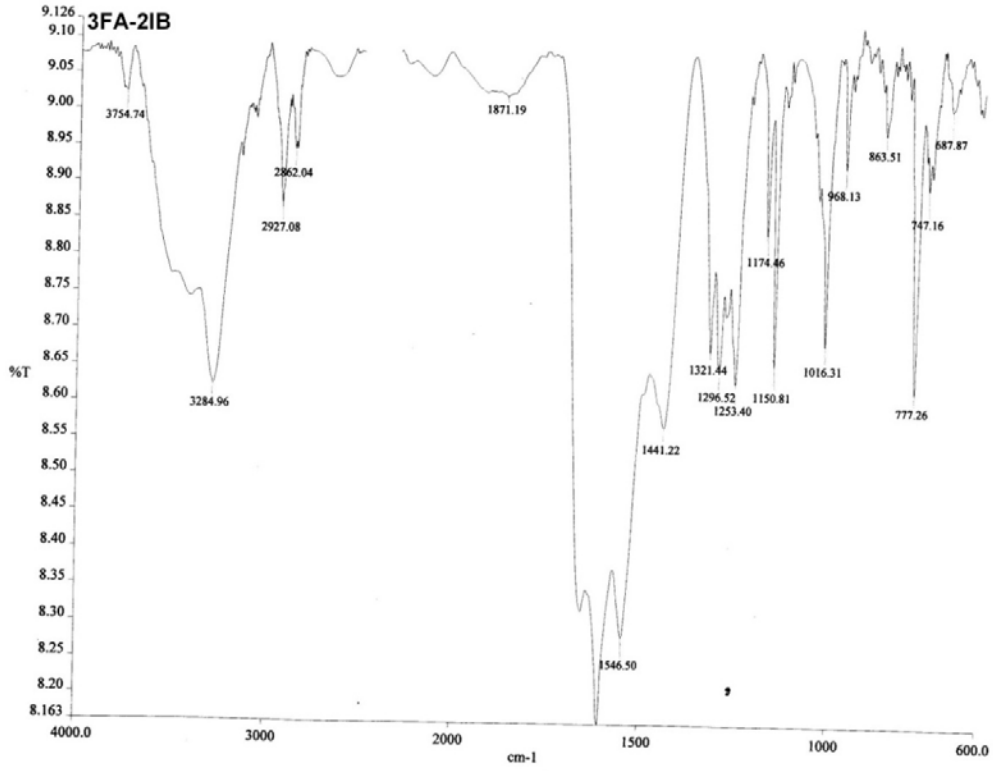


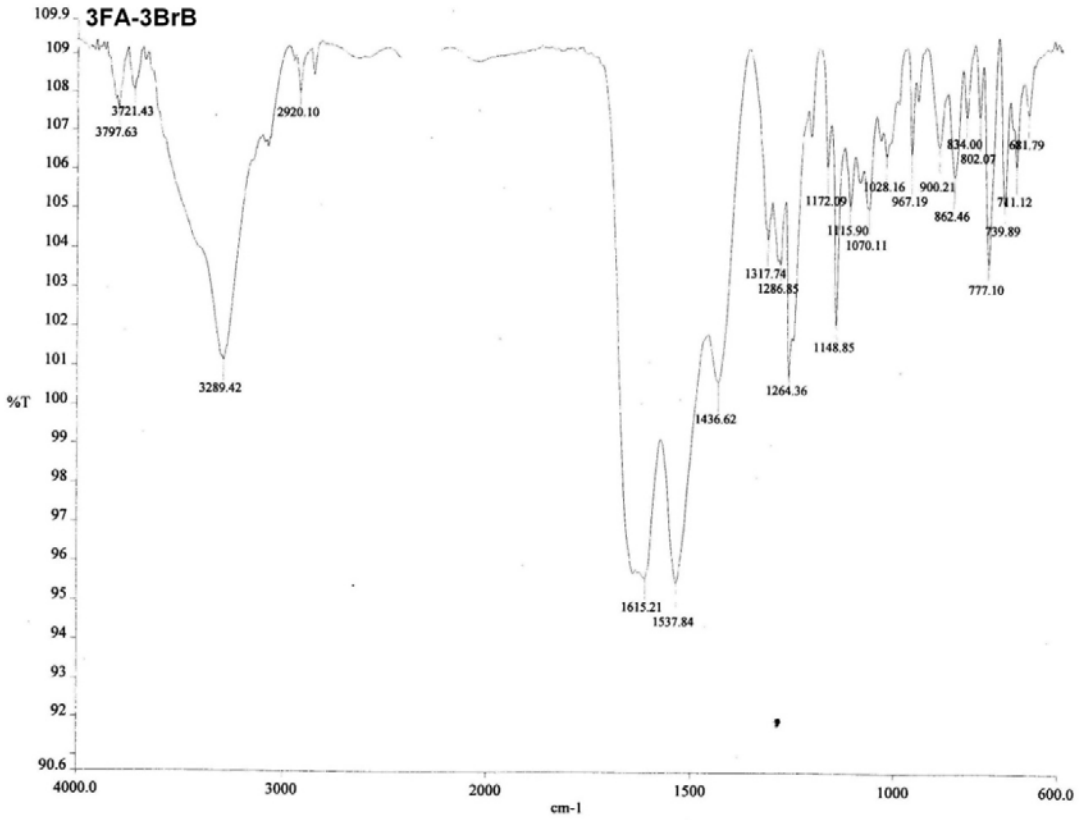
The stretching frequency of 2FA-2IB is listed below as text as shown in figures whereas for the remaining samples, the similar trends observed with small variation as shown in figures.

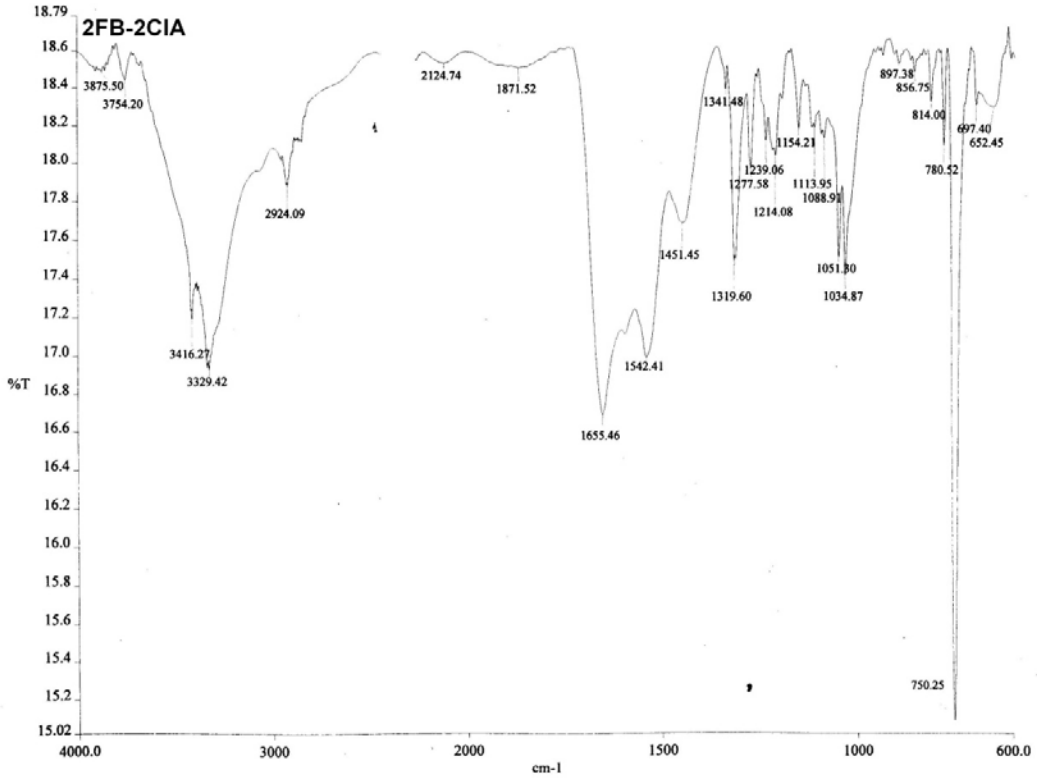
IR (Neat) cm-1: 3271.83 (N-H str), 2918.90 (ArC-H str), 1668.59 (C=O amide str), 1519.71, 1318.00 (C=C str), 1299.25 (C-N str), 1196.40 (Ar-F str).

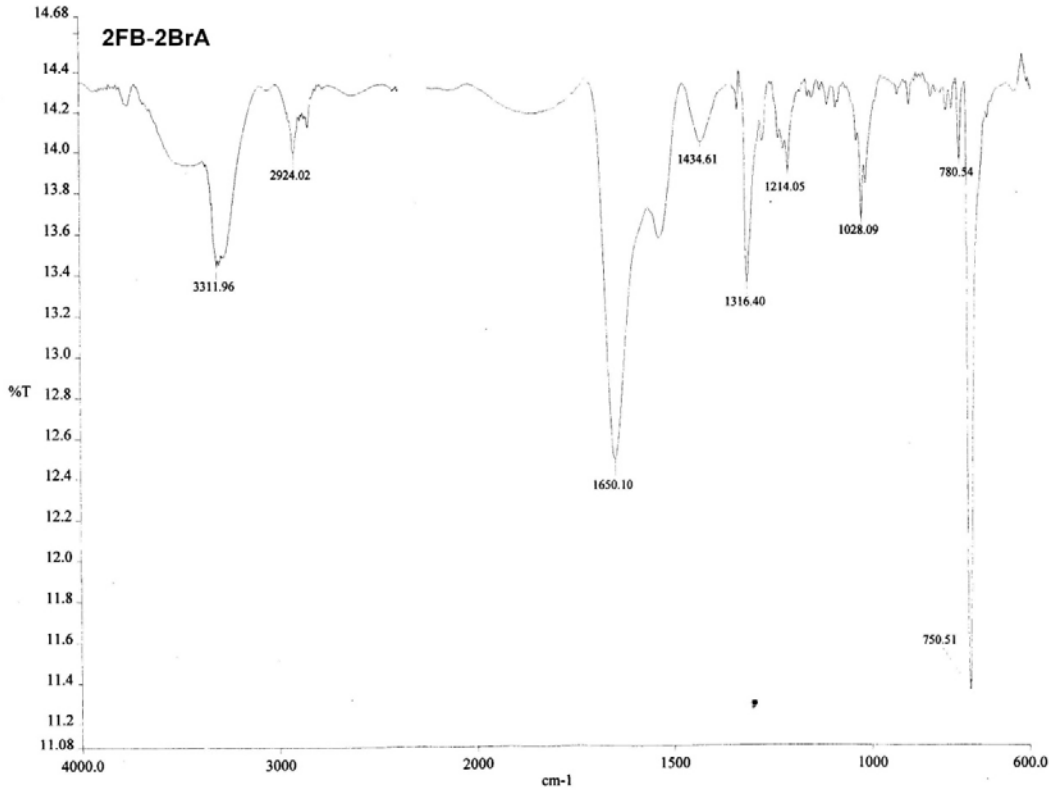


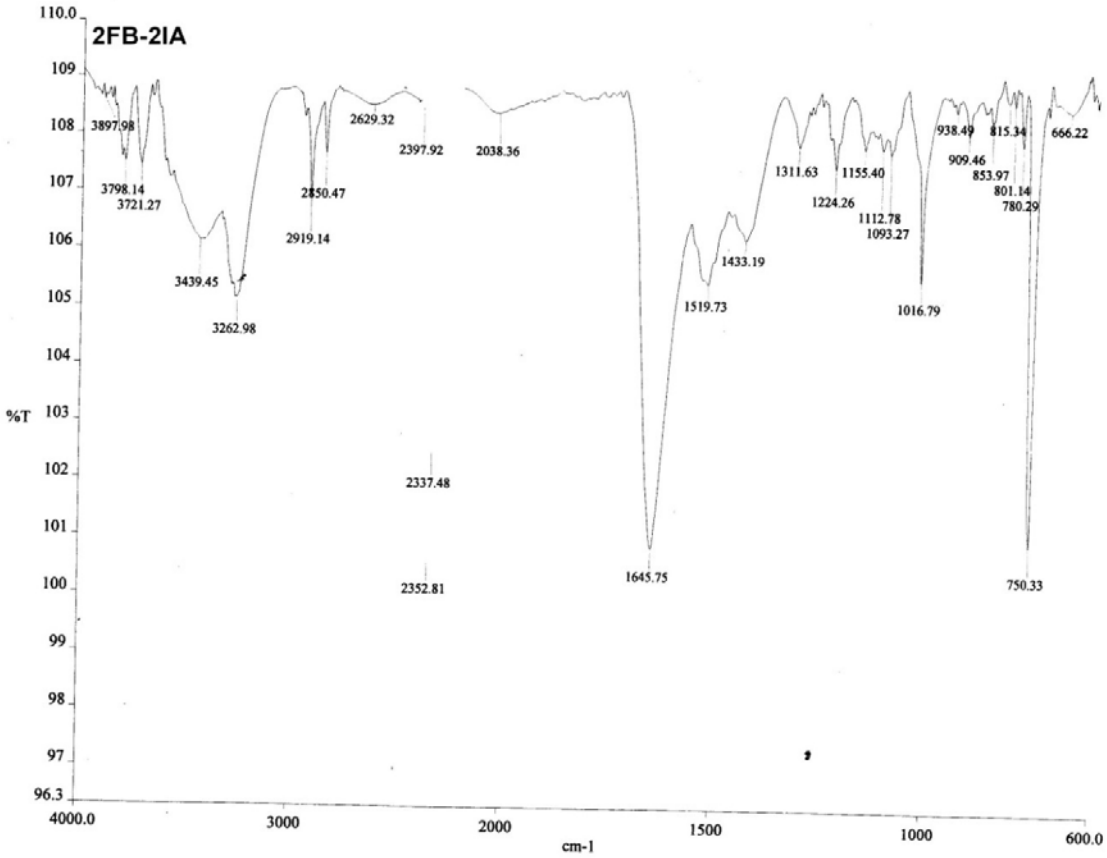


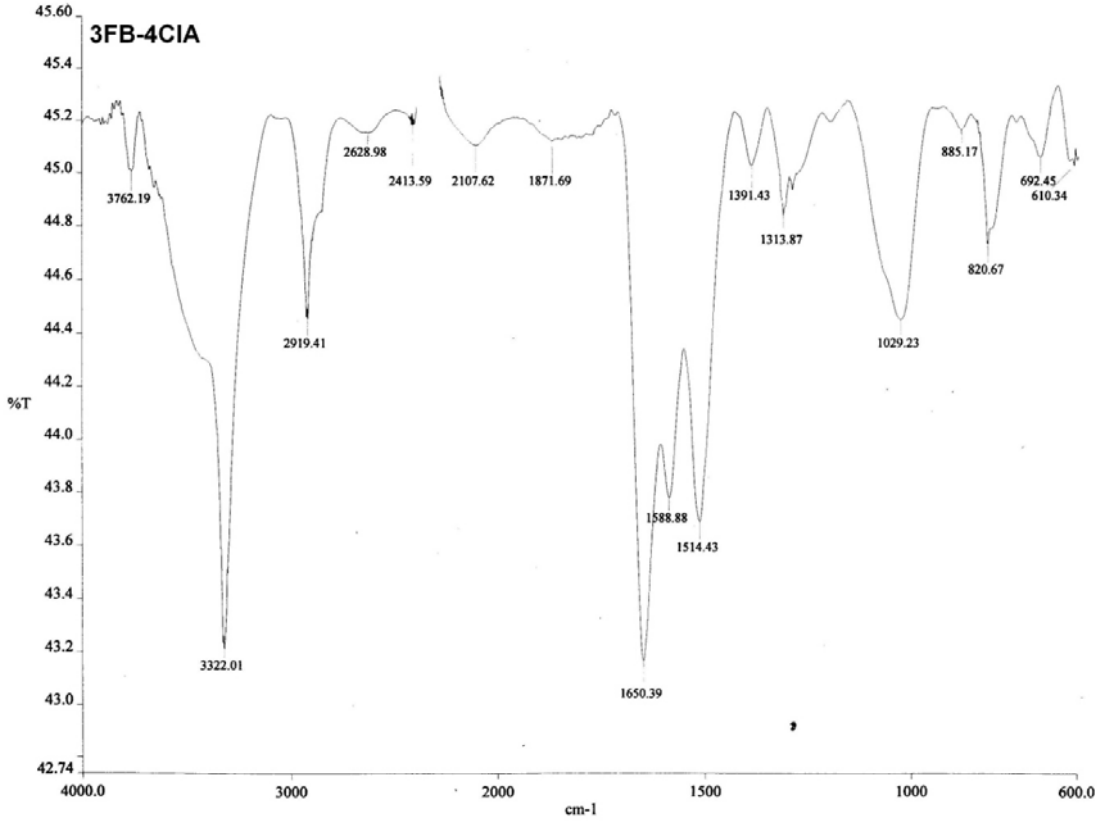


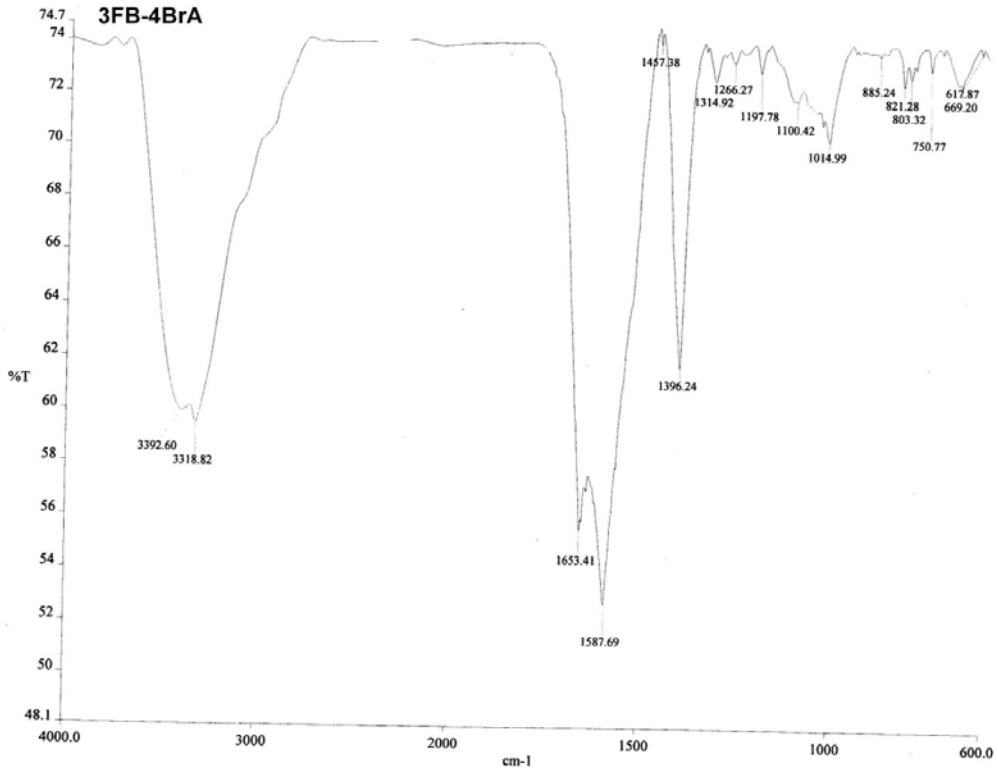




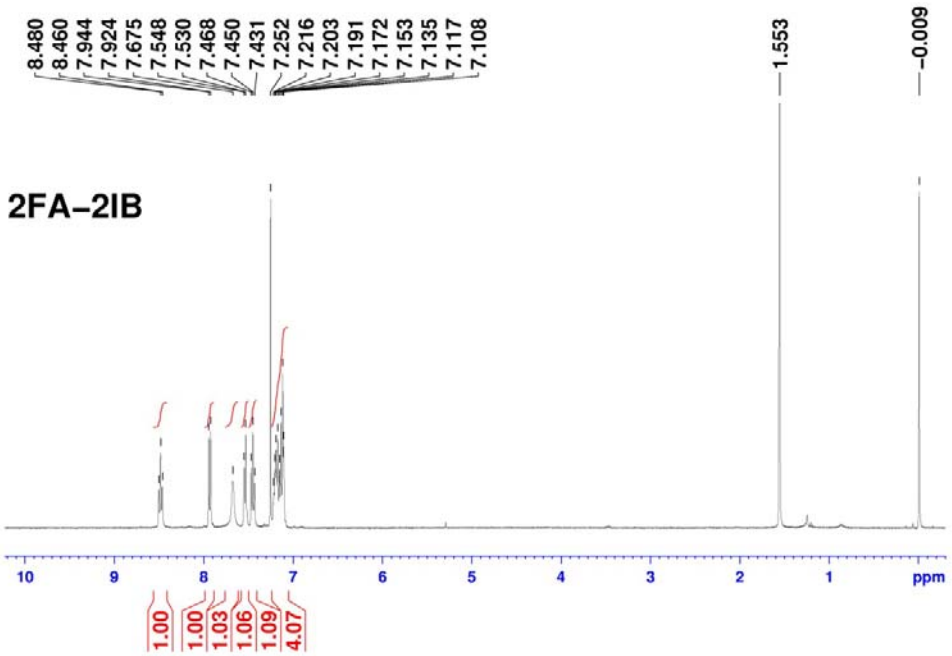




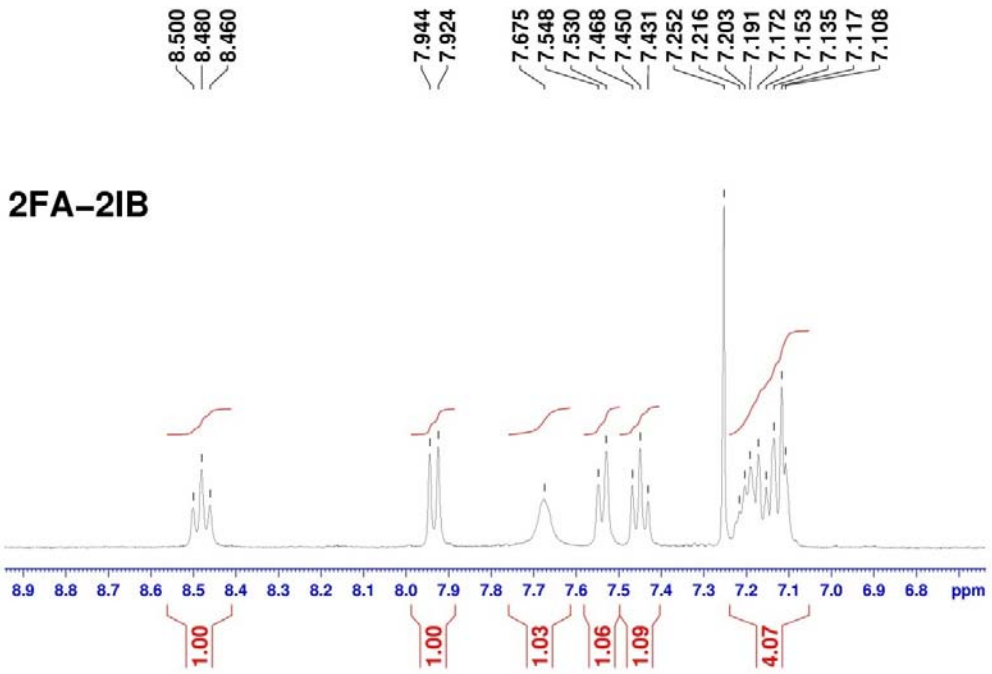


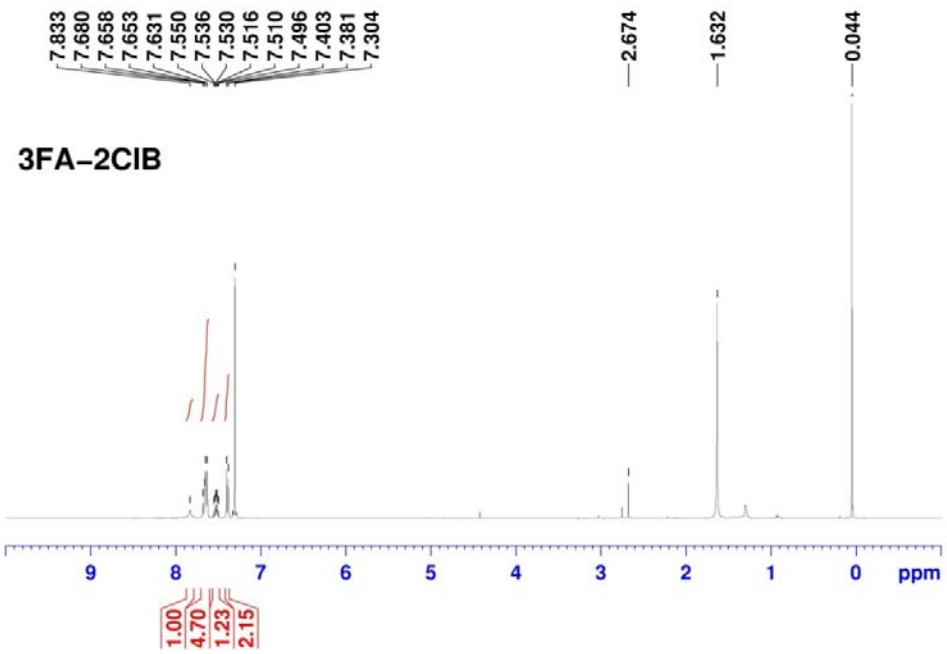


^{1}HNMR- Of samples provides evidence for purity of the samples before crystallization.



The magnified regions (6.5-9 ppm) have been shown for better clarity





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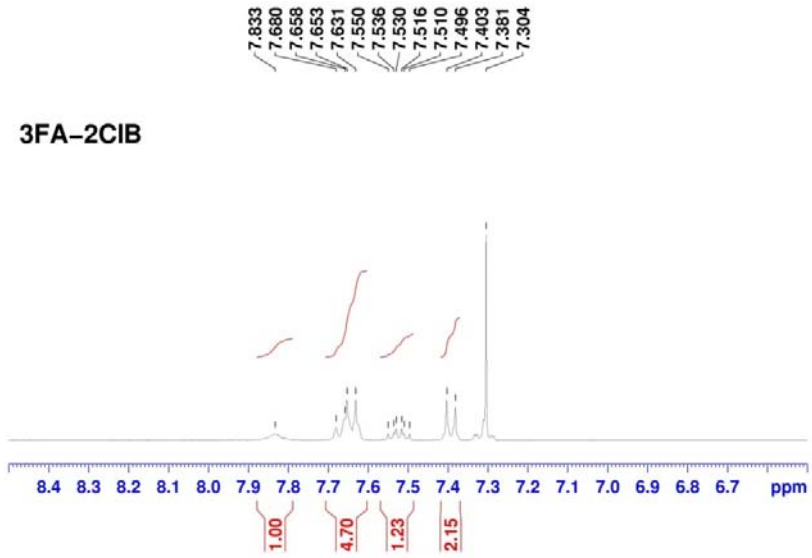

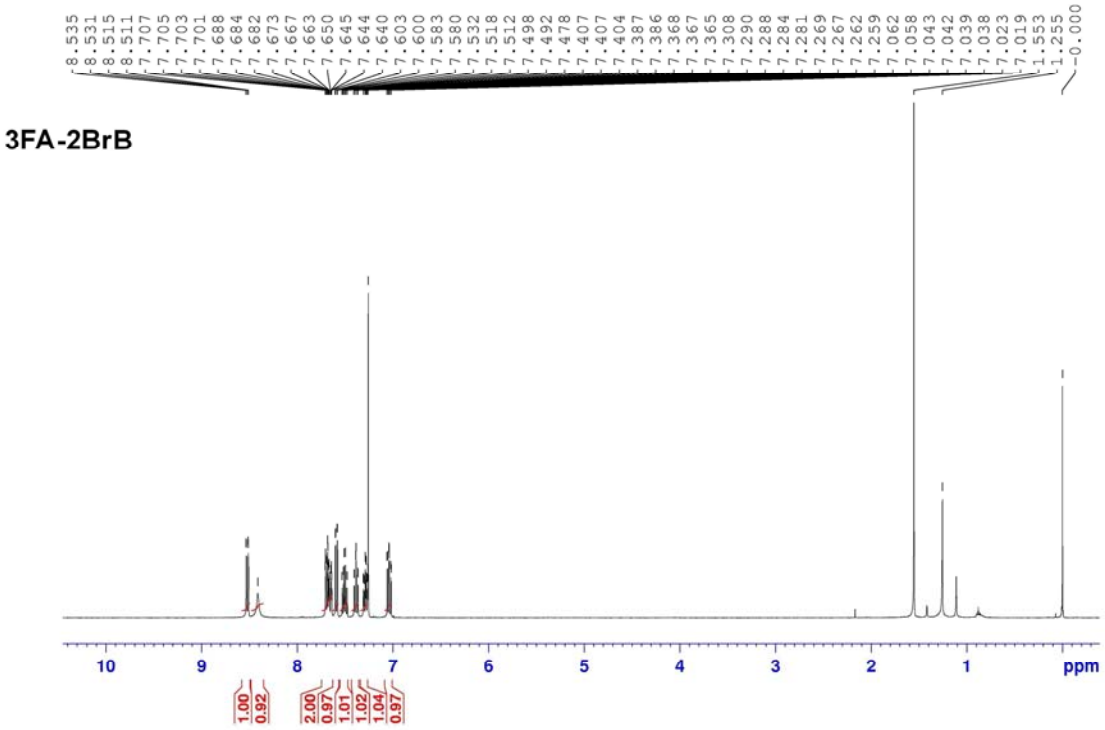

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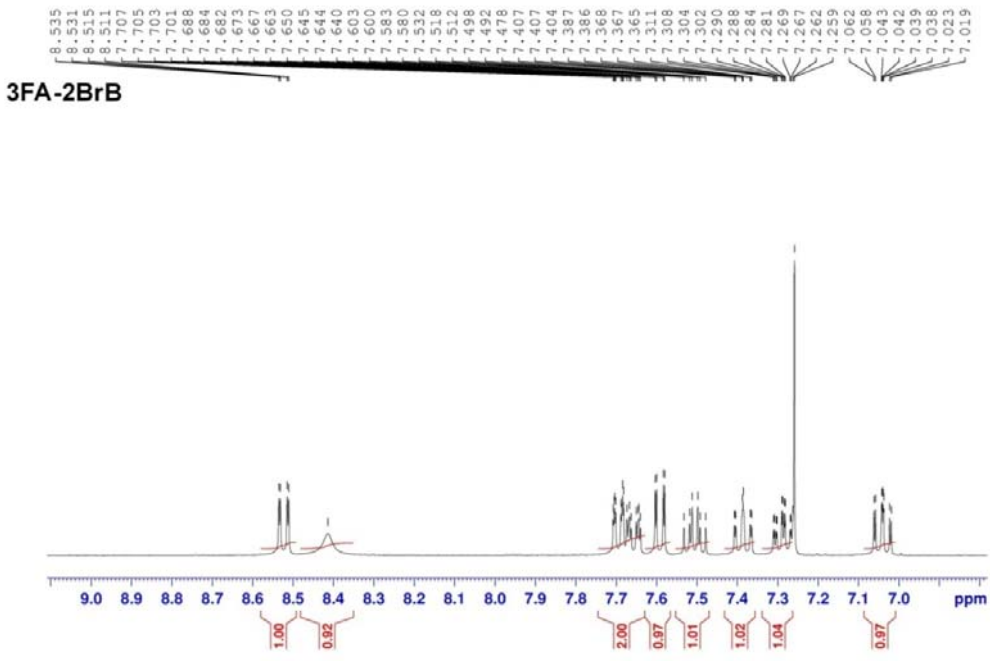

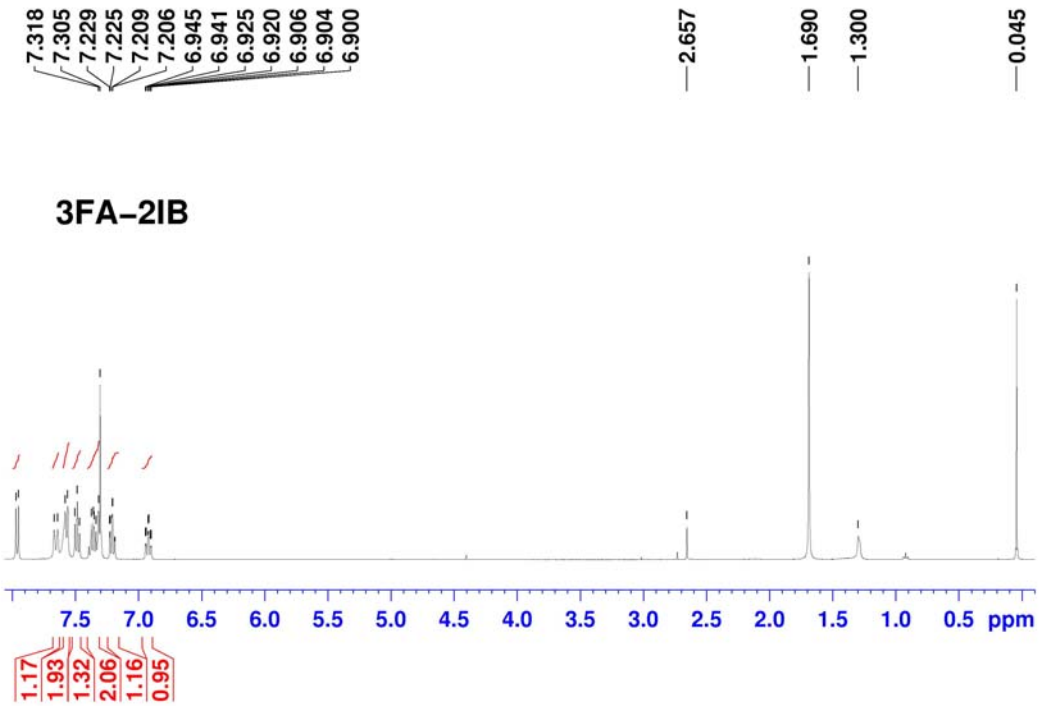

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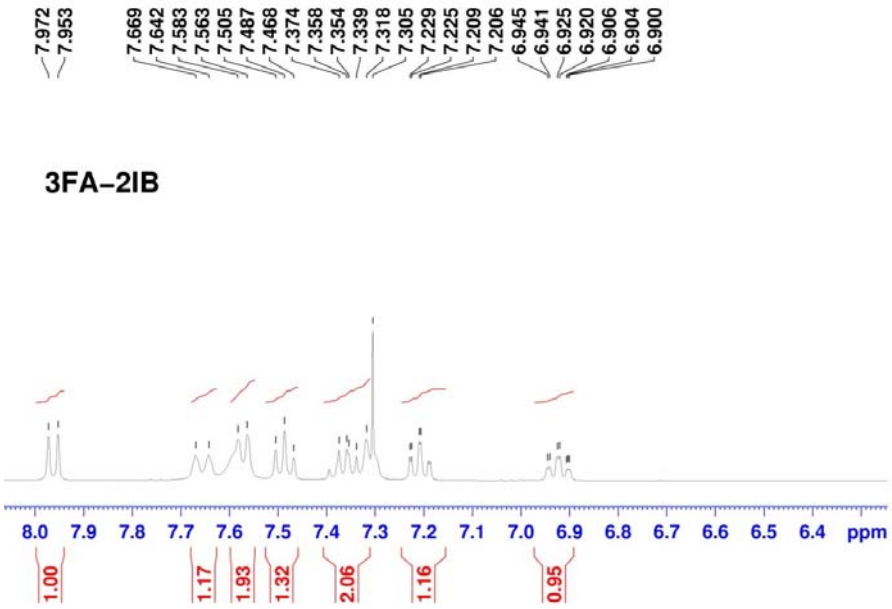

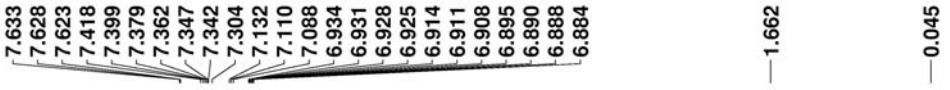

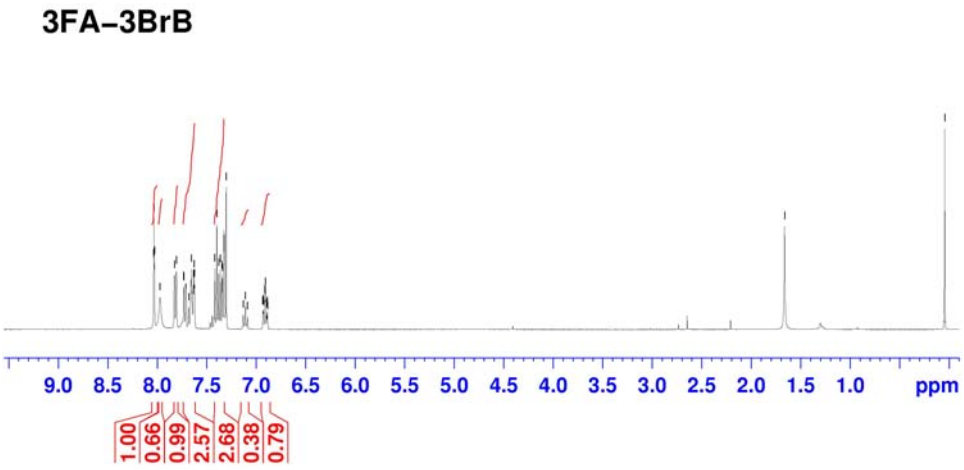

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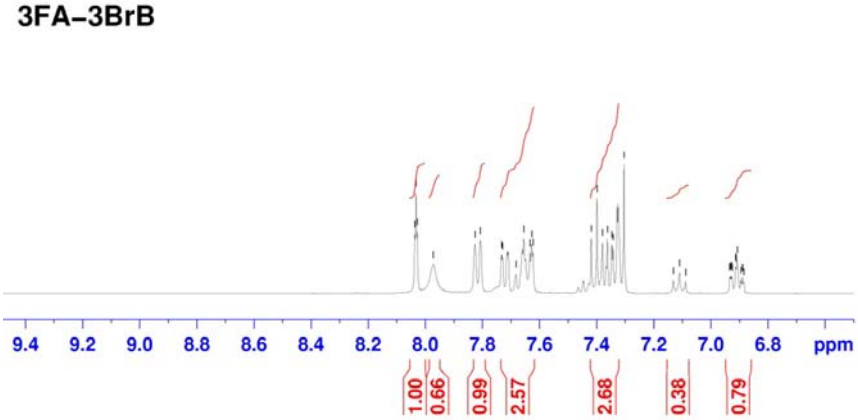
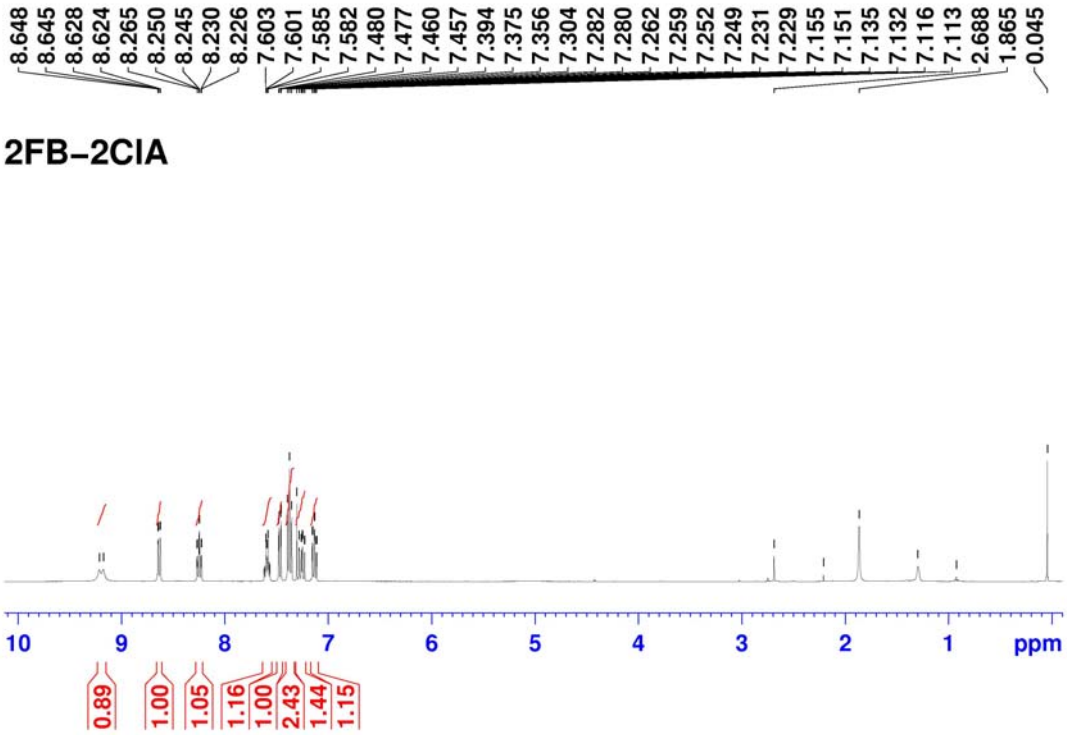
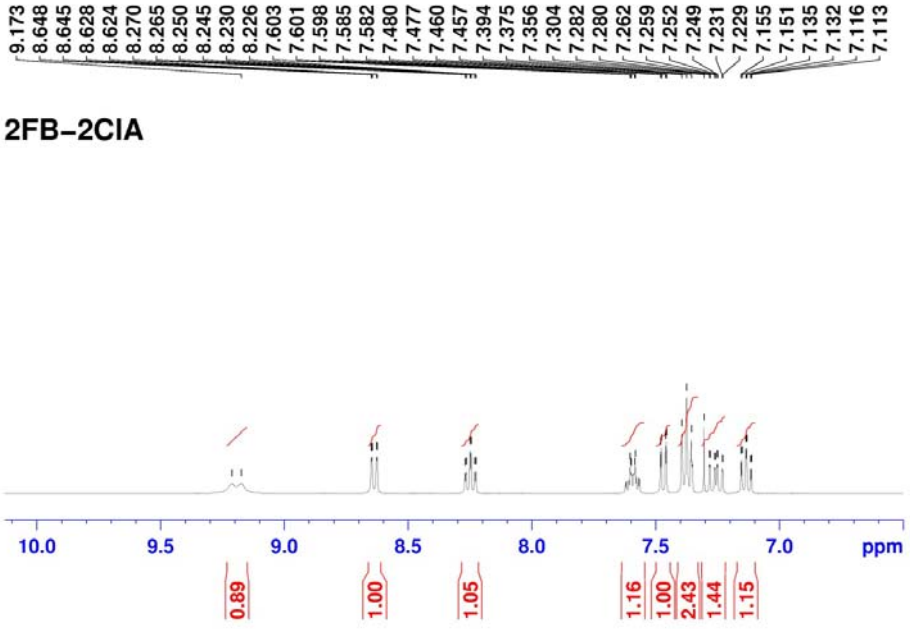
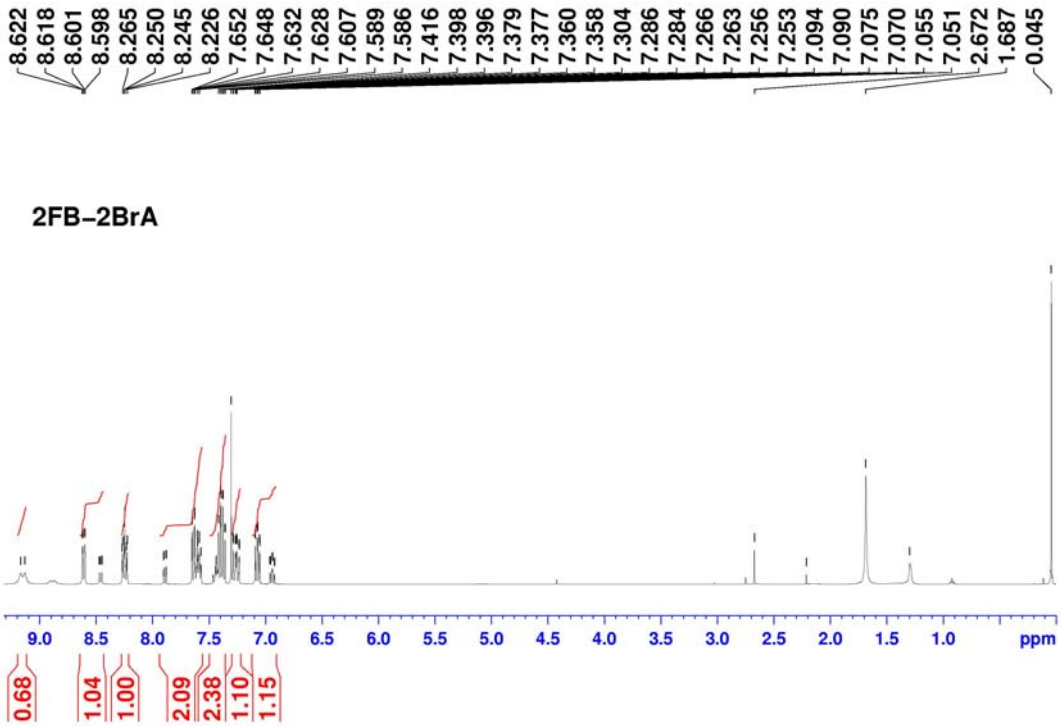




The magnified regions (6.5-9 ppm) have been shown for better clarity





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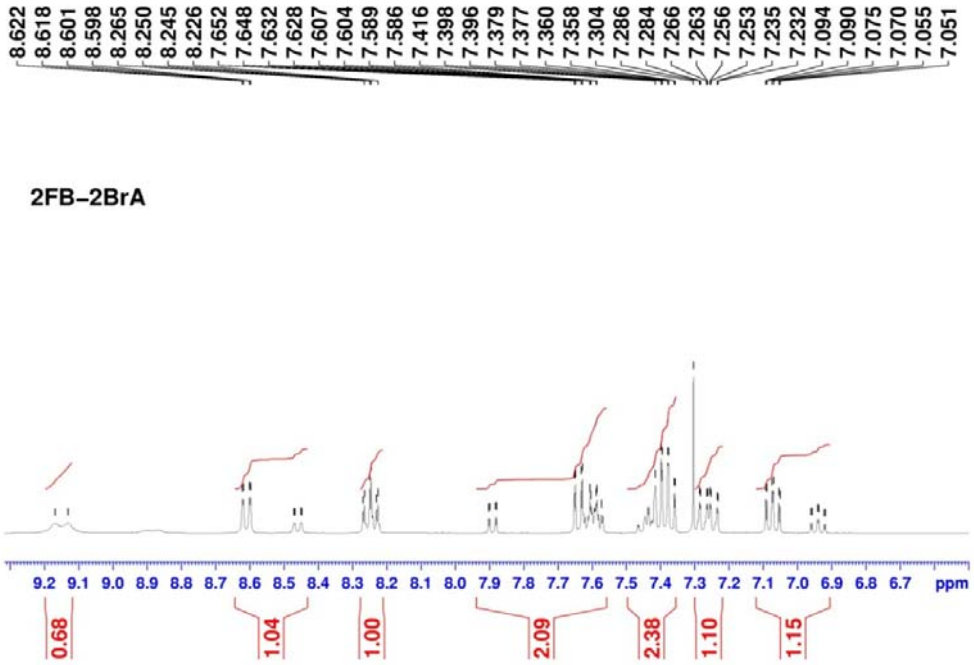

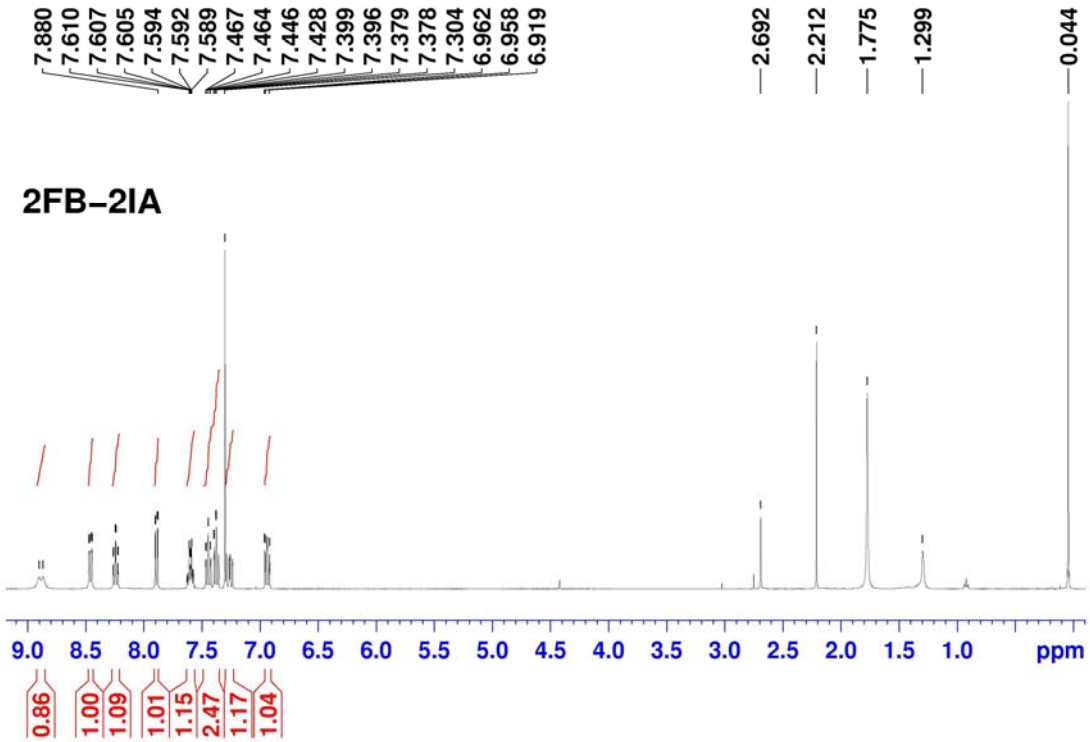

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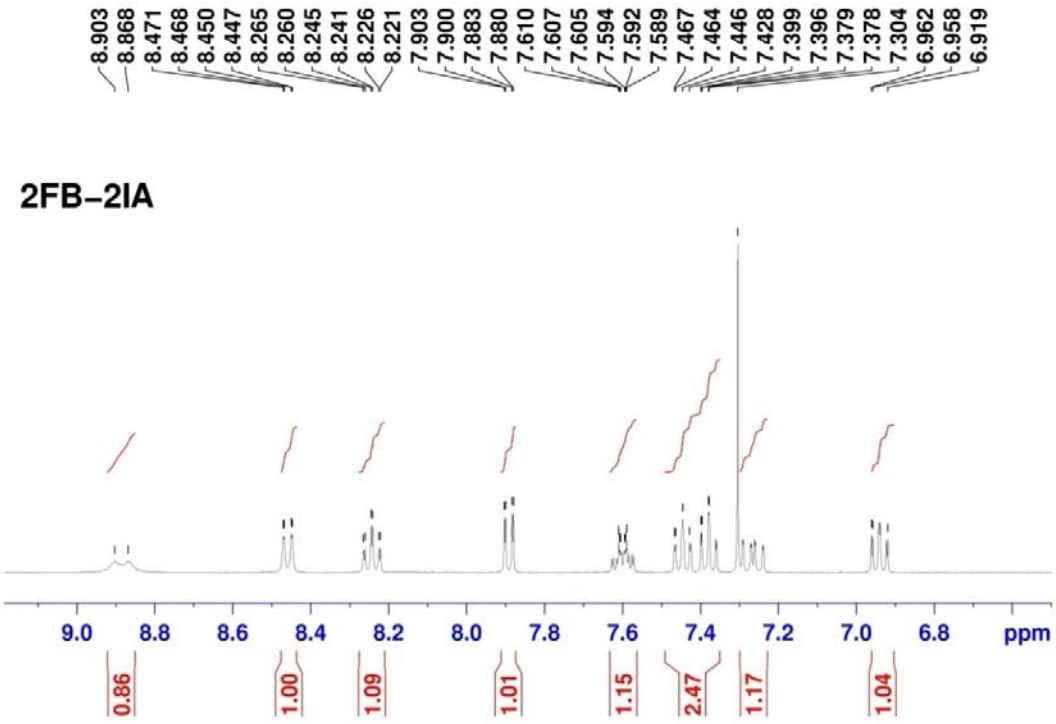

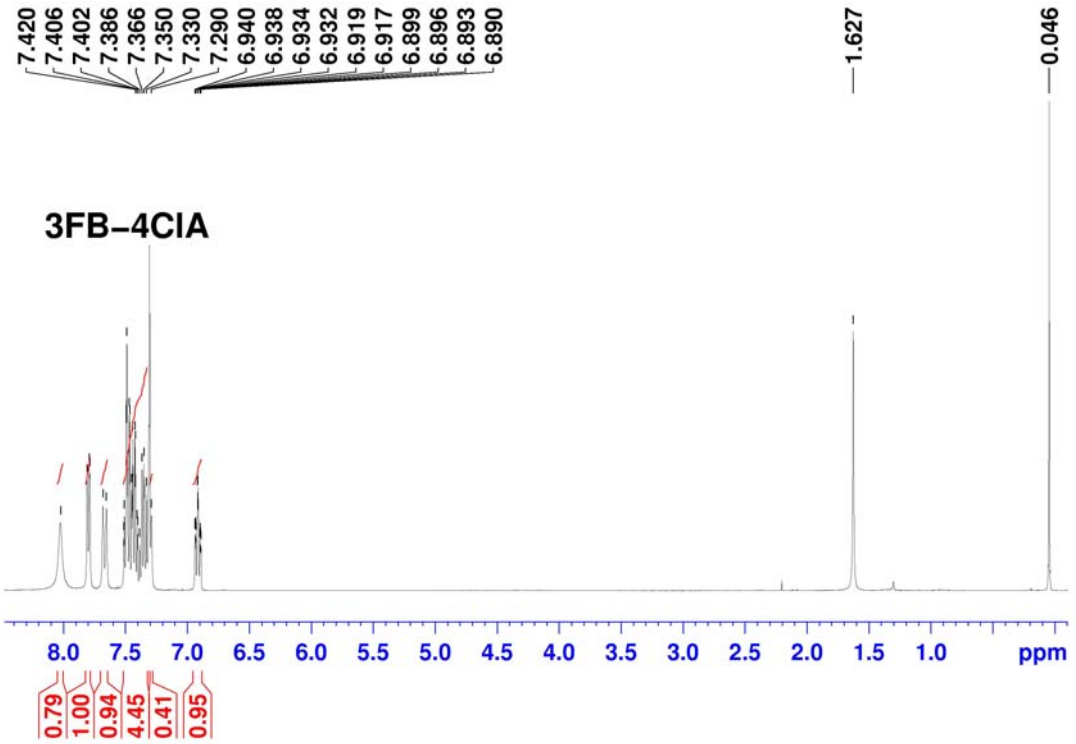

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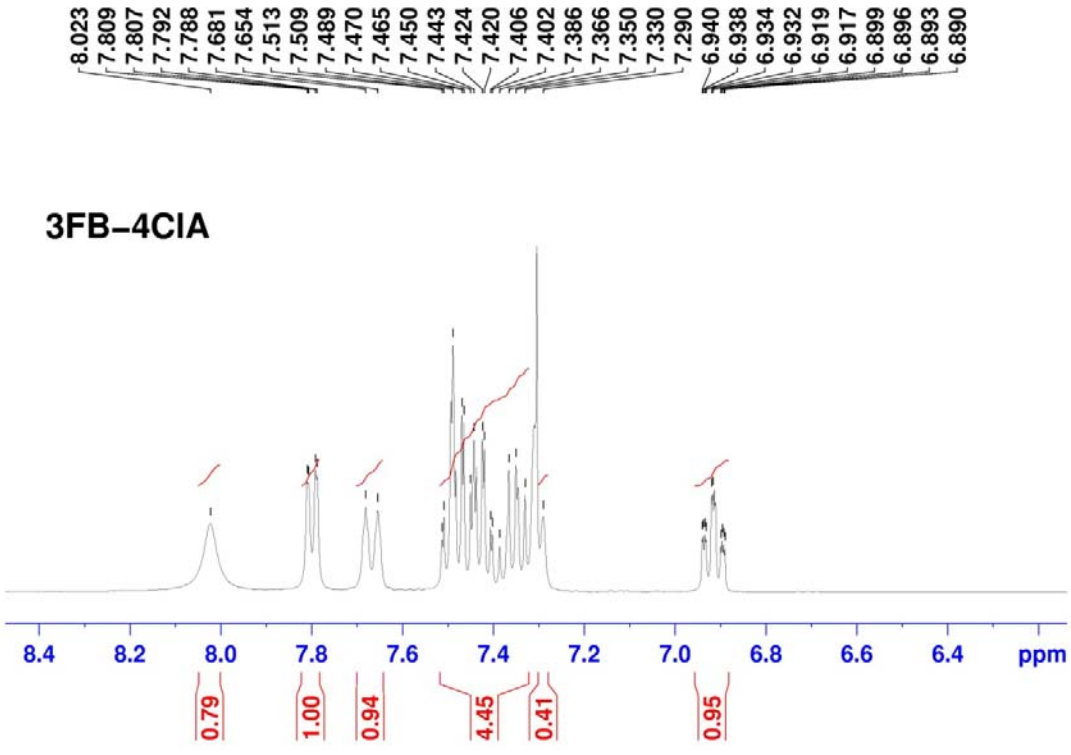

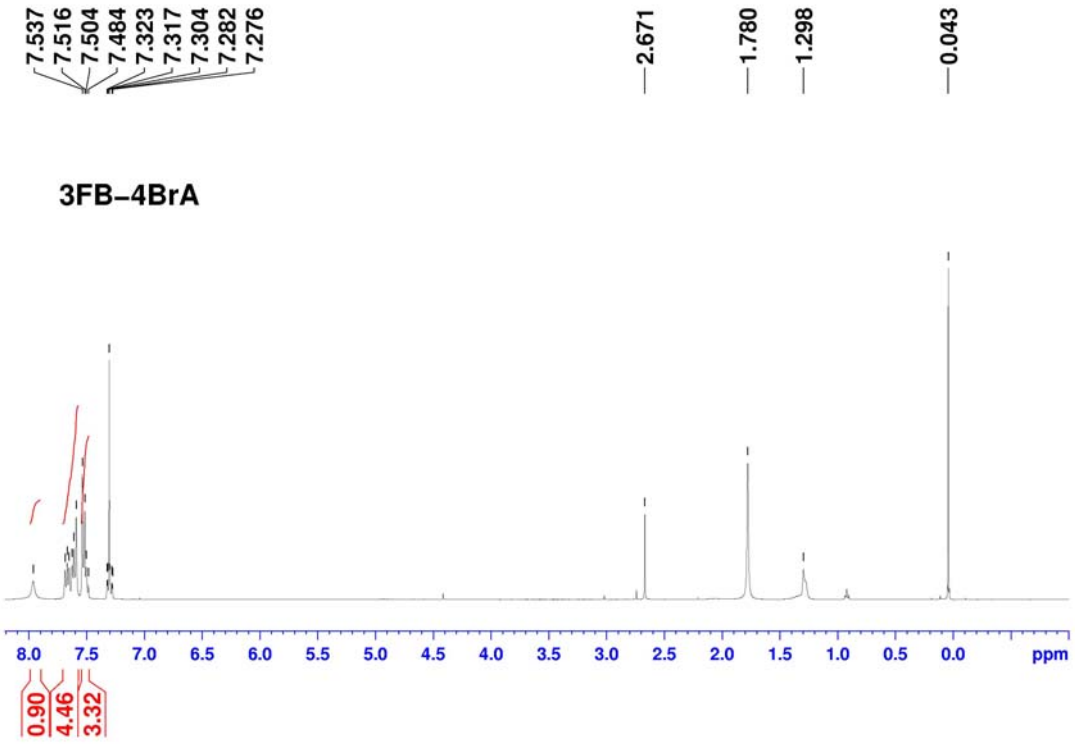

The magnified regions (6.5-9 ppm) have been shown for better clarity