

Supplementary Information

Synthesis of fluorinated ferrocene derivatives for their thermal behavior and their *in silico* studies in designing of potential breast cancer inhibitors

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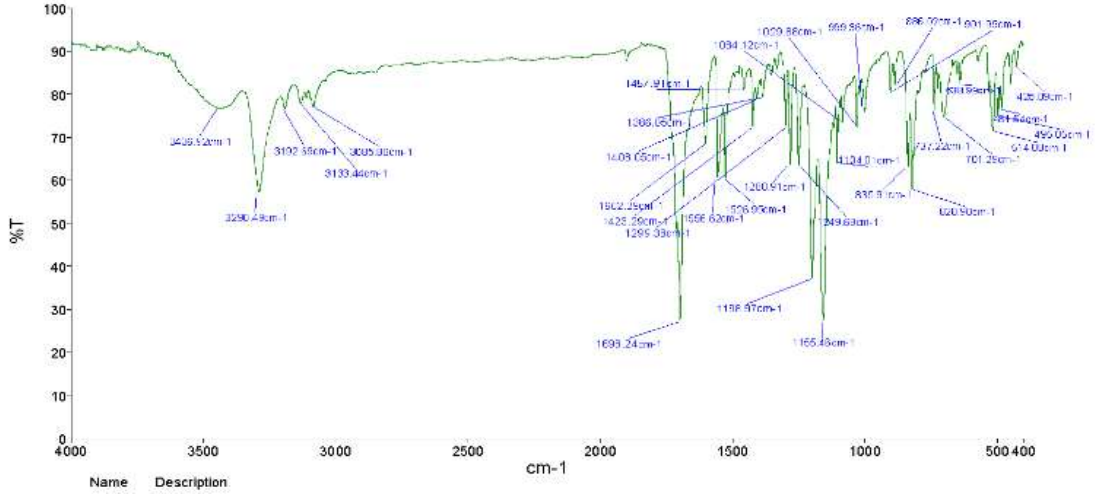
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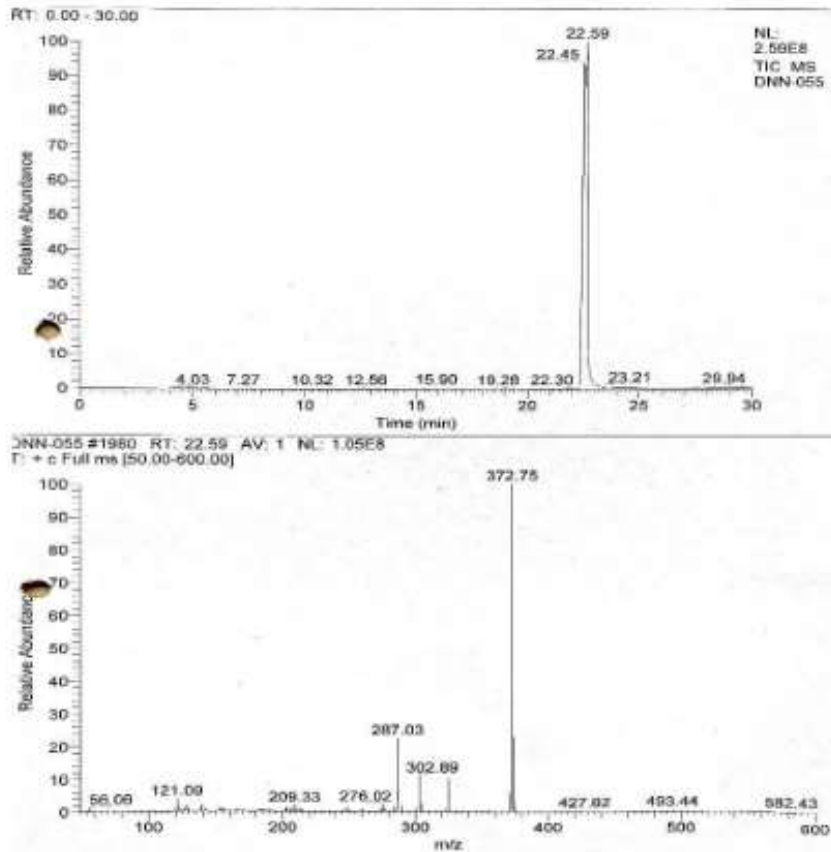
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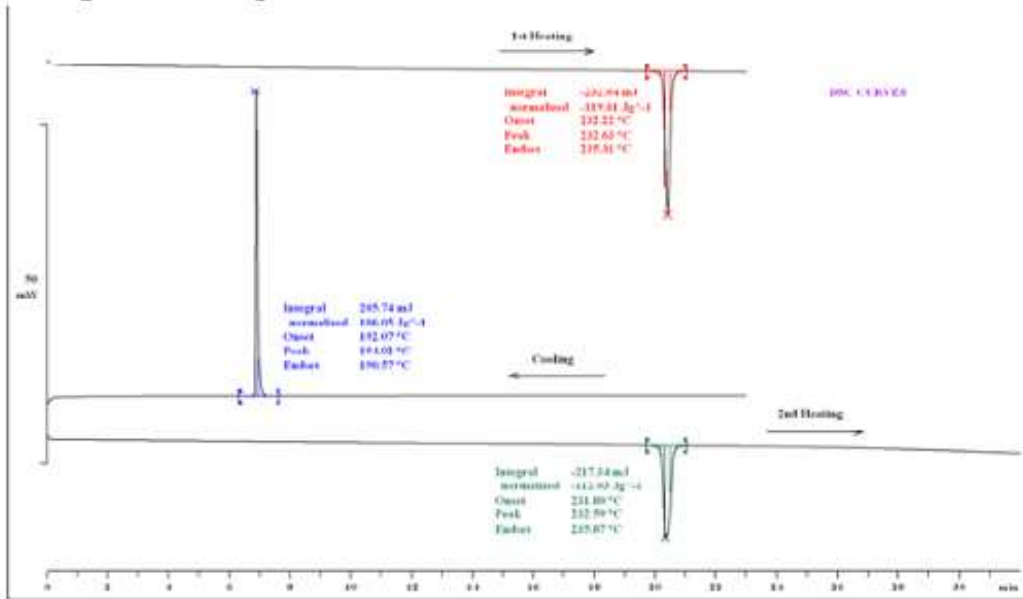
1) Spectral data of Compound No. 04 IR Spectra of Compound No. 04



Mass Spectra of Compound No. 04

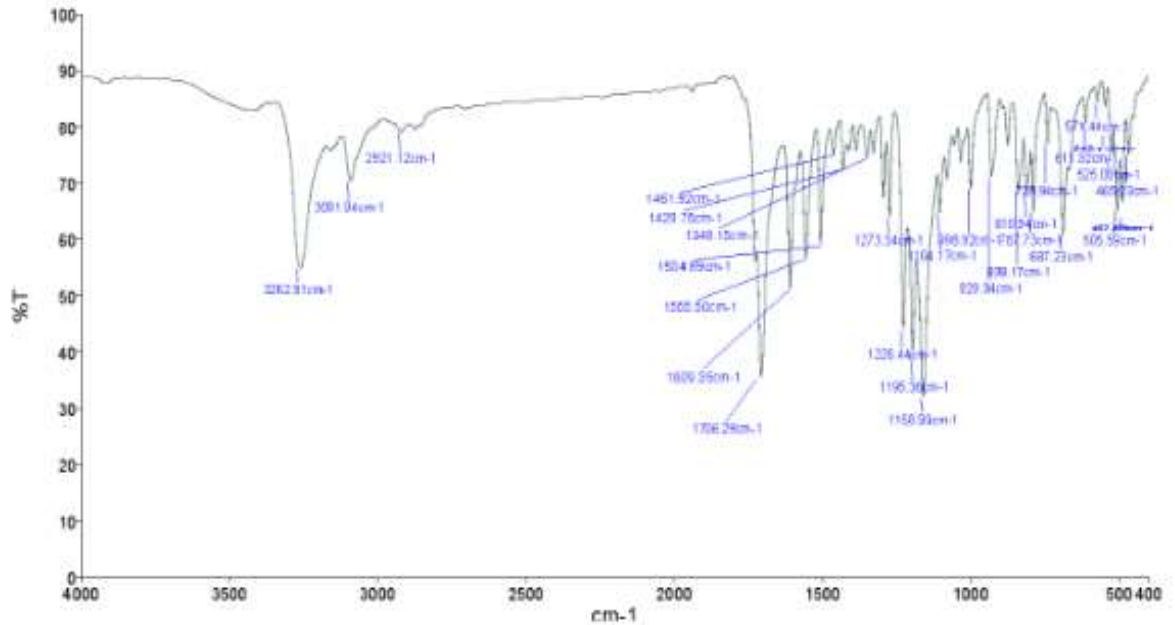


DSC thermogram of compound 04

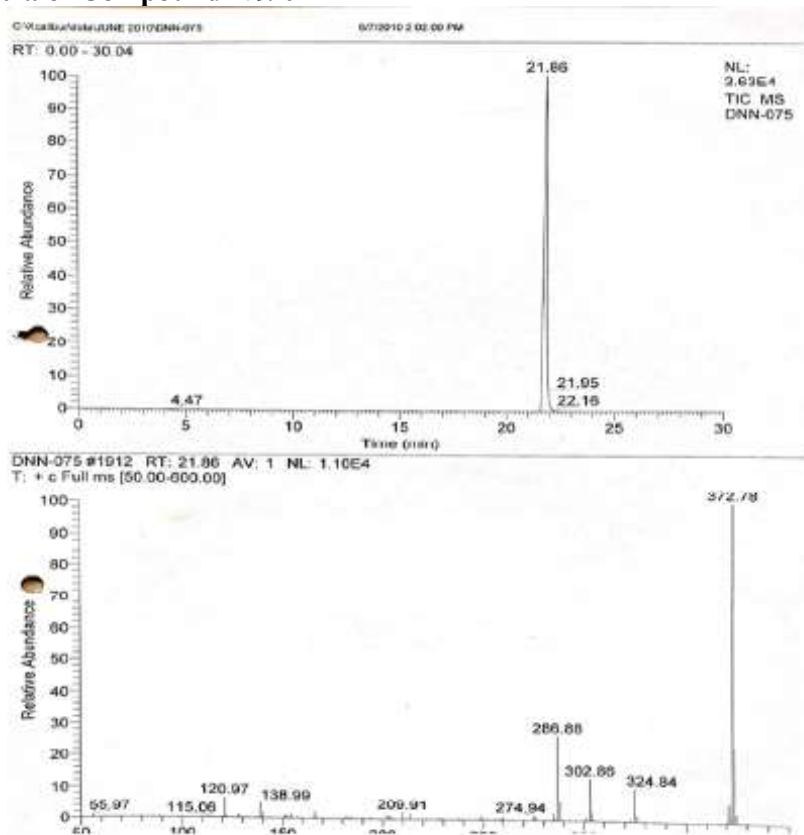


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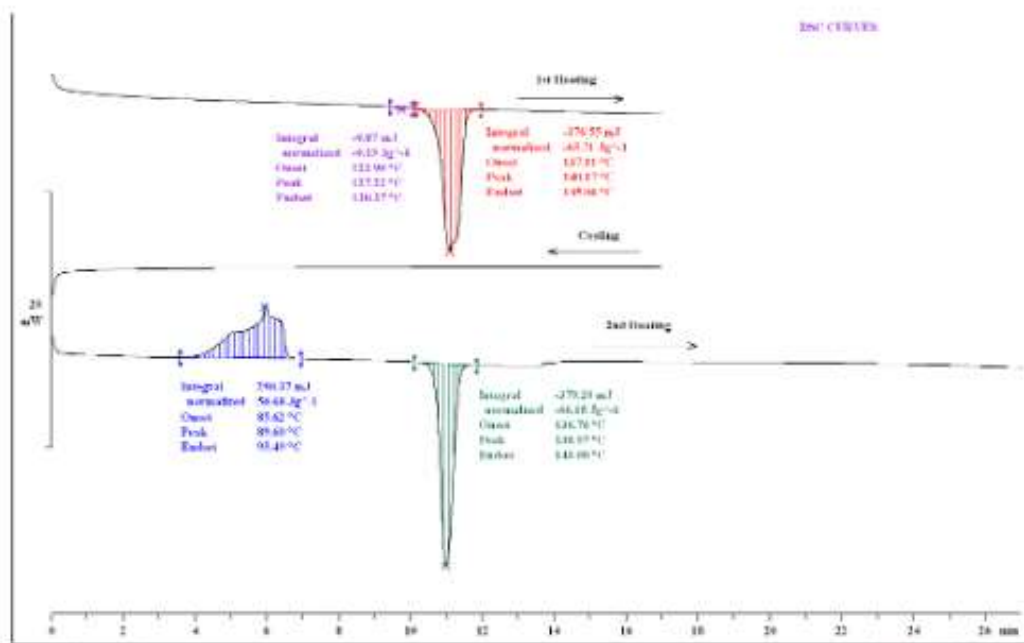
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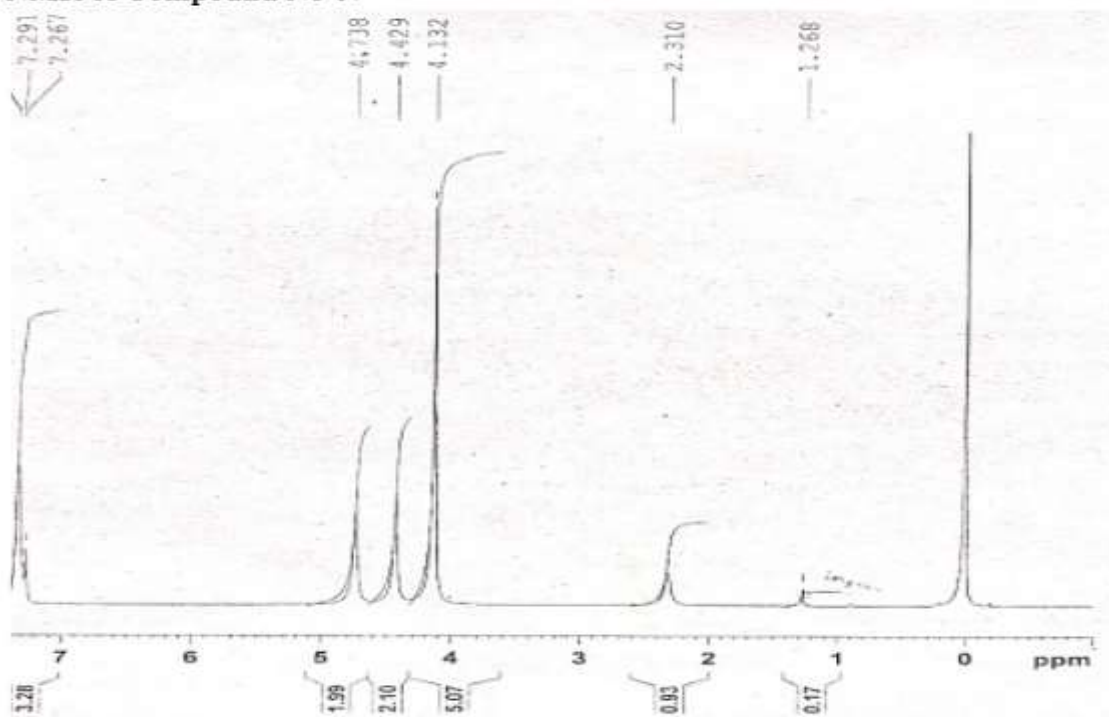
Mass Spectra of Compound No. 07



DSC thermogram of compound 07

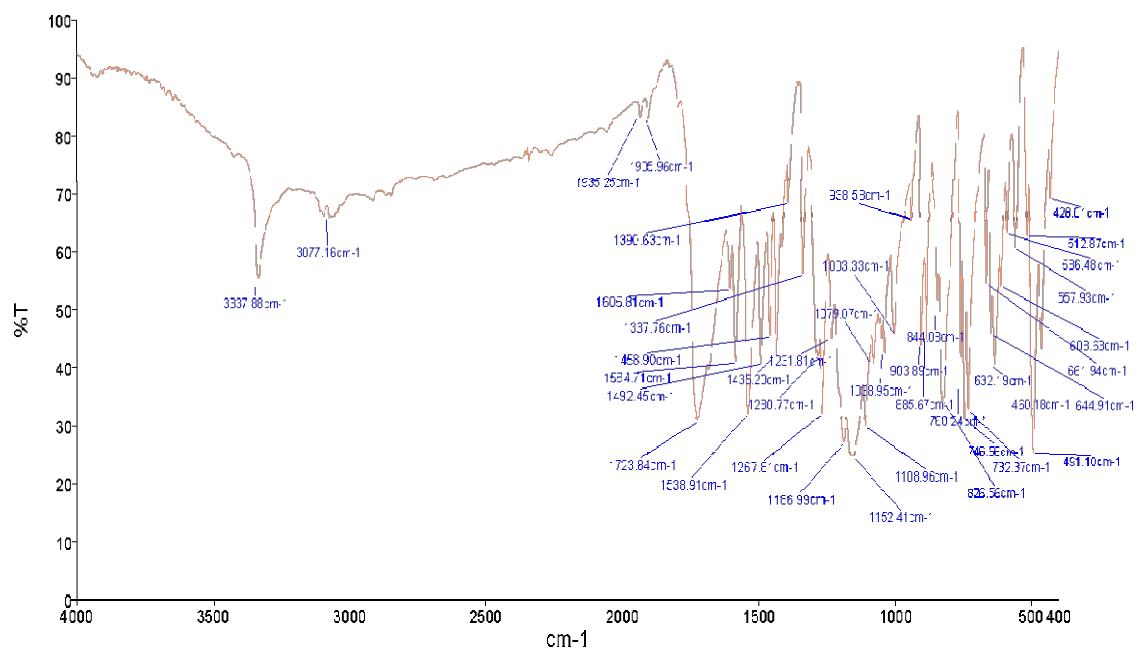


¹H NMR of Compound No 07

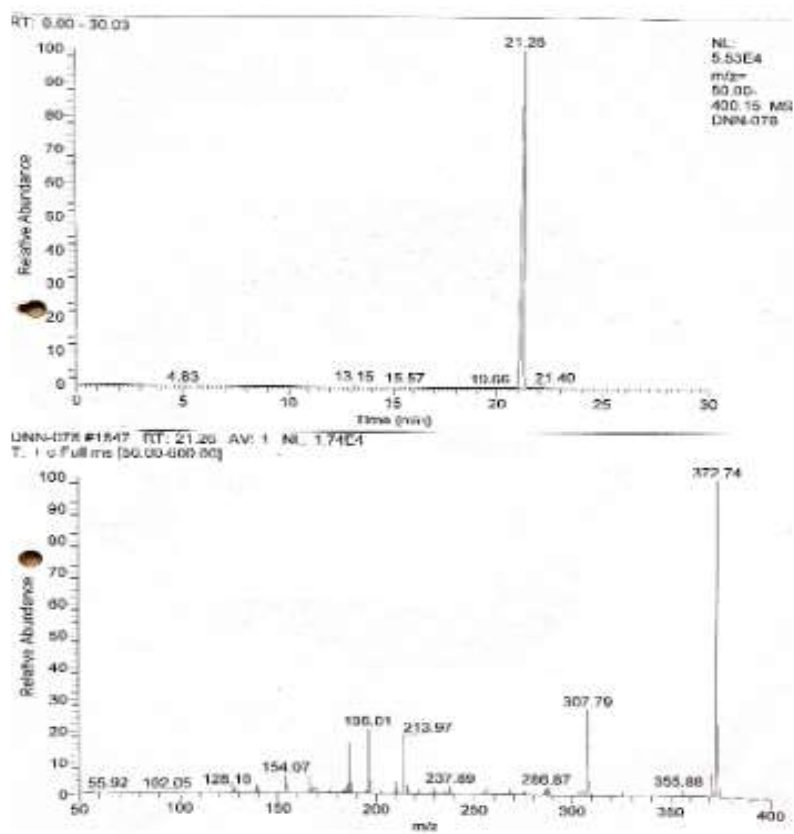


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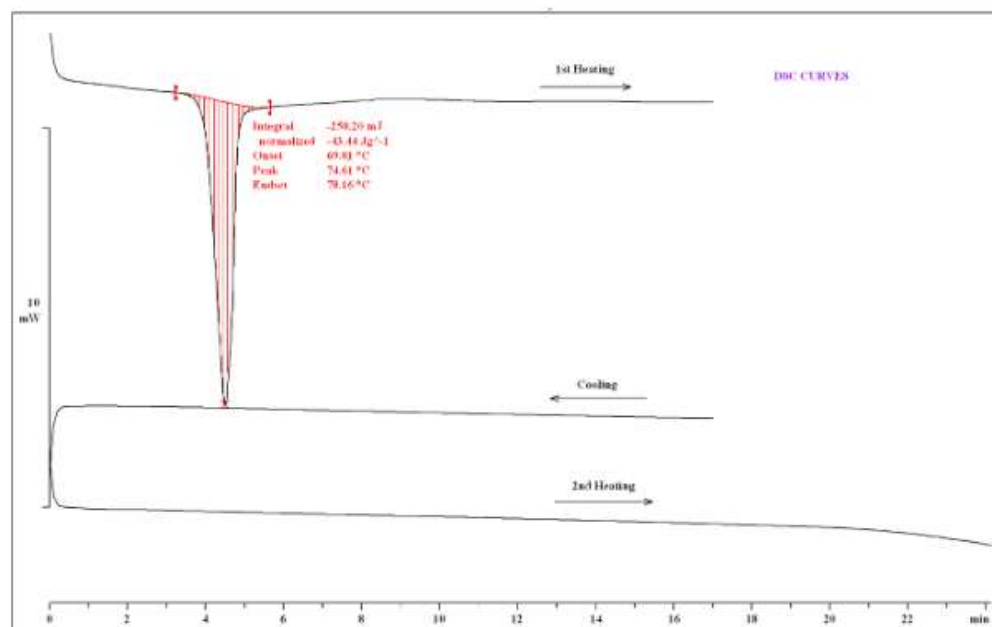
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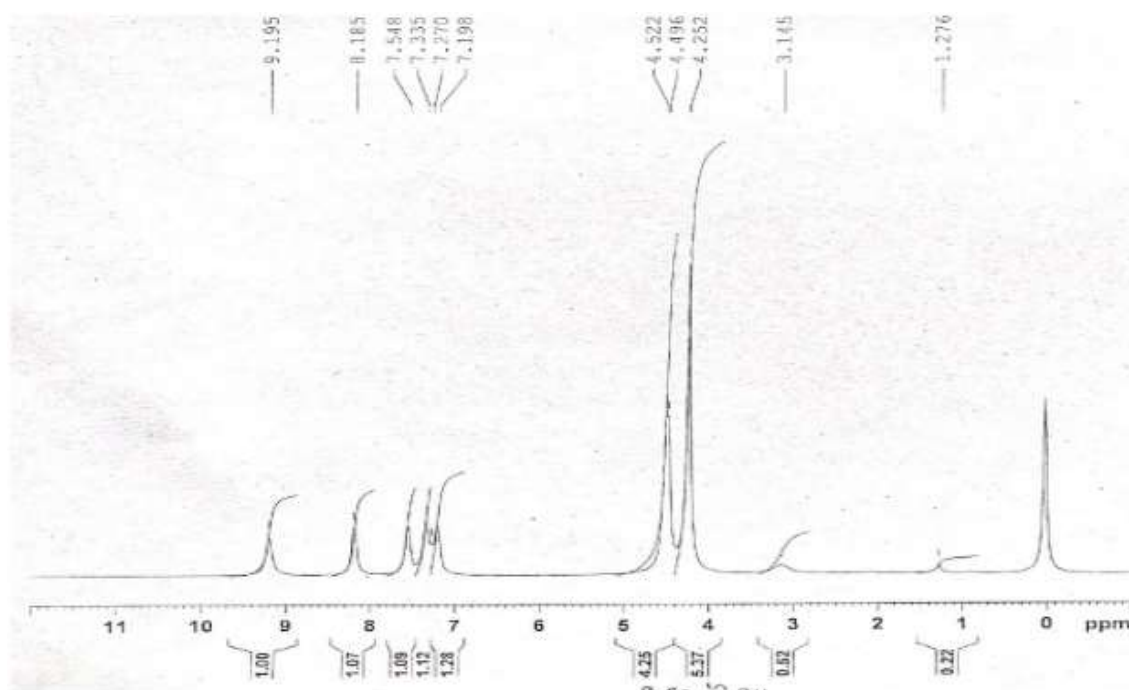
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DSC Spectra of Compound No. 10

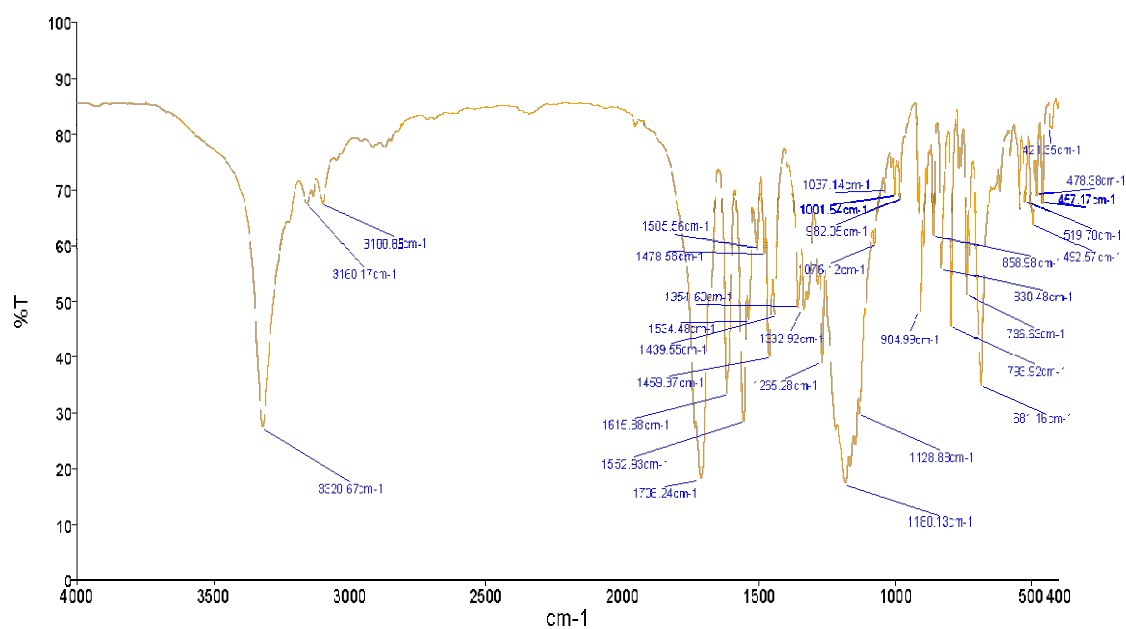


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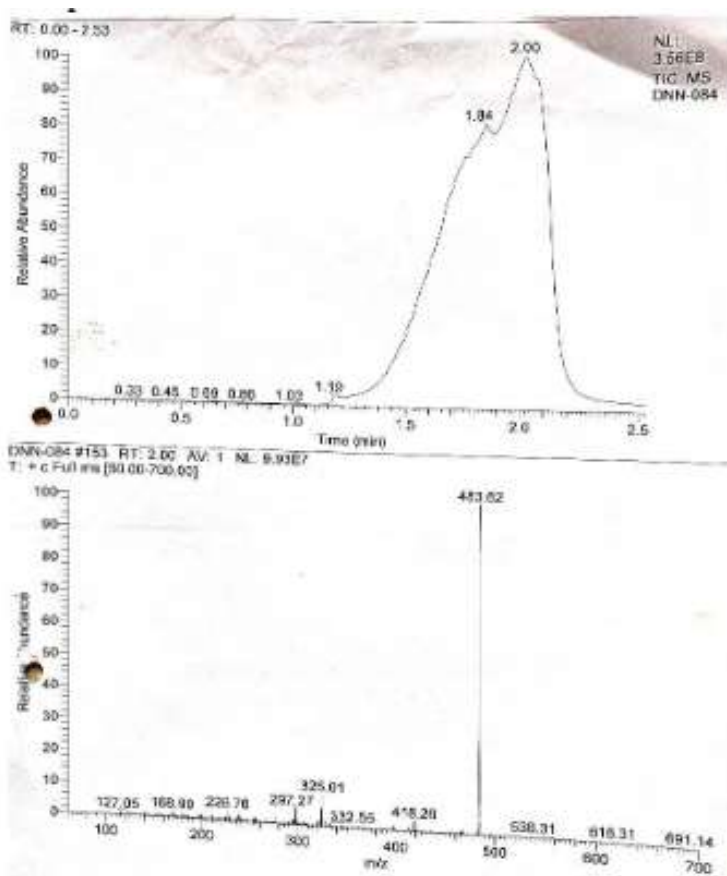


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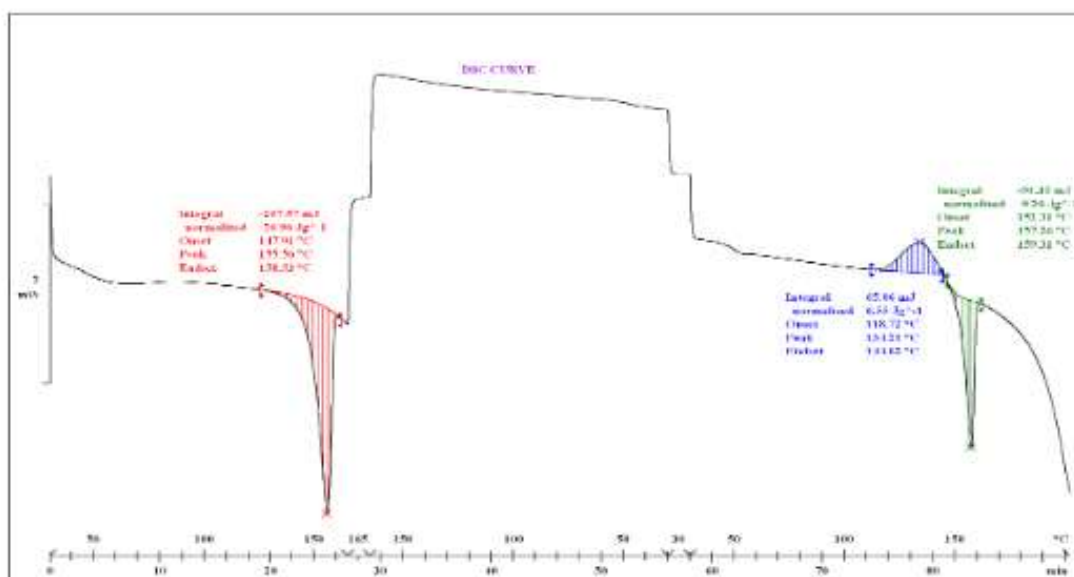
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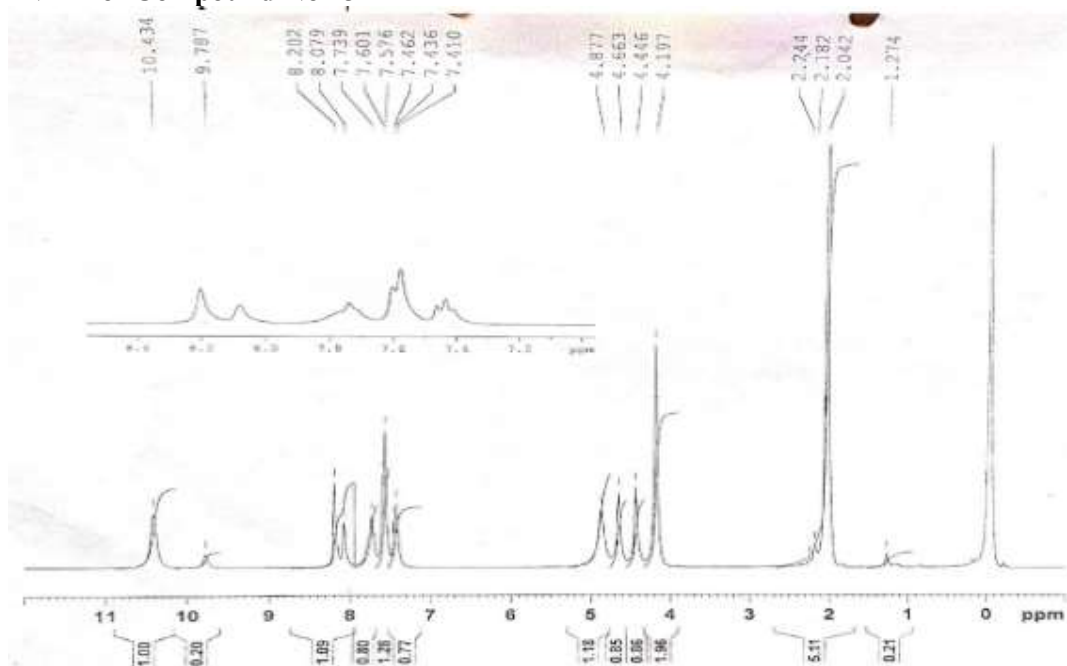
Mass Spectra of Compound No. 13



DSC Spectra of Compound No. 13

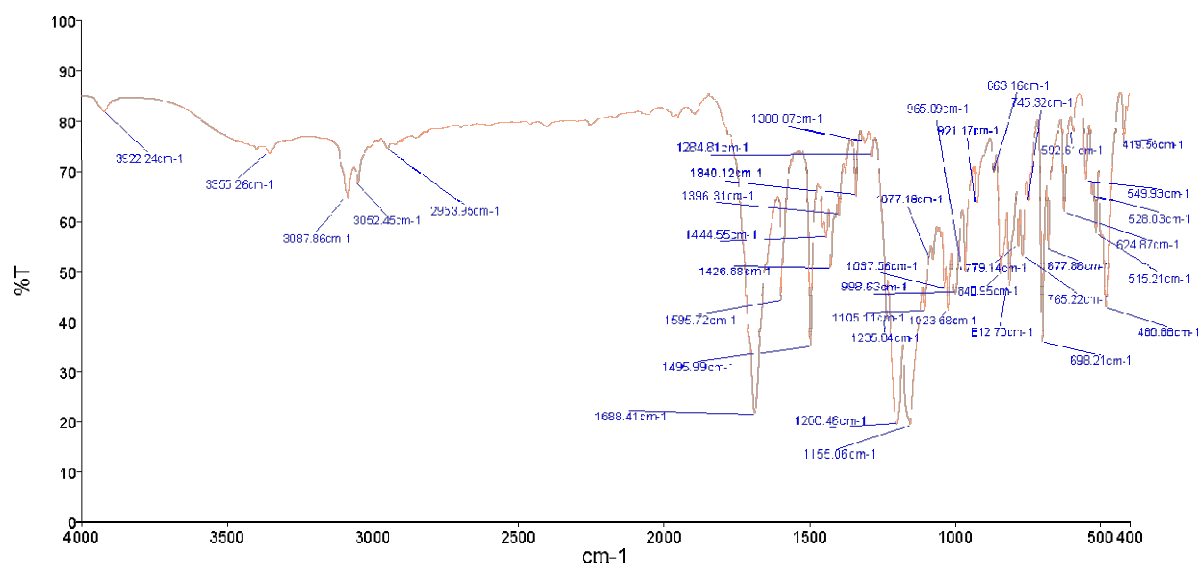


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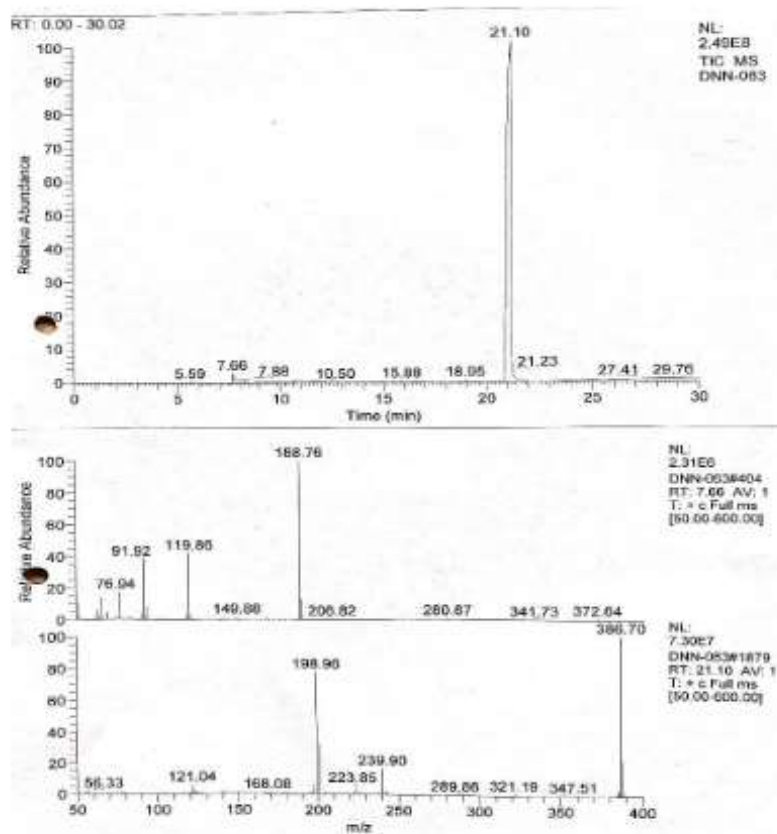


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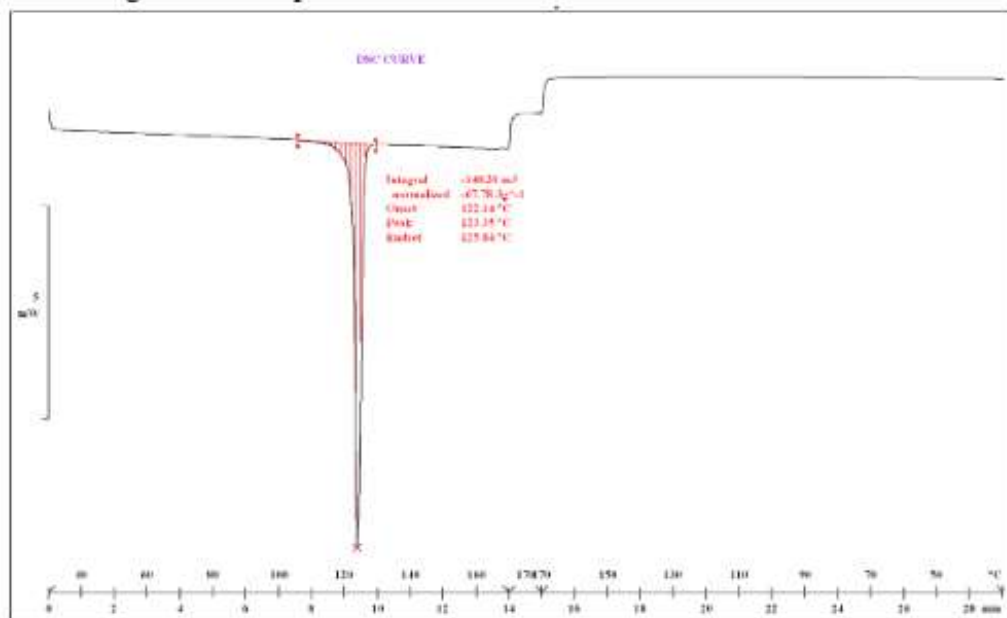
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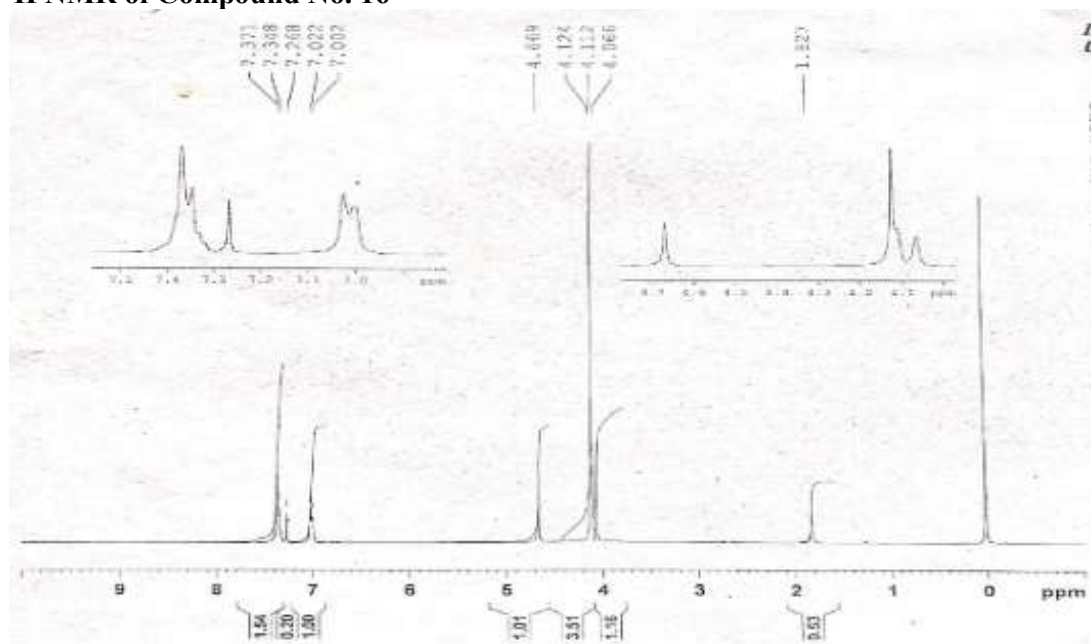
Mass Spectra of Compound No. 16



DSC Thermogram of Compound No. 16

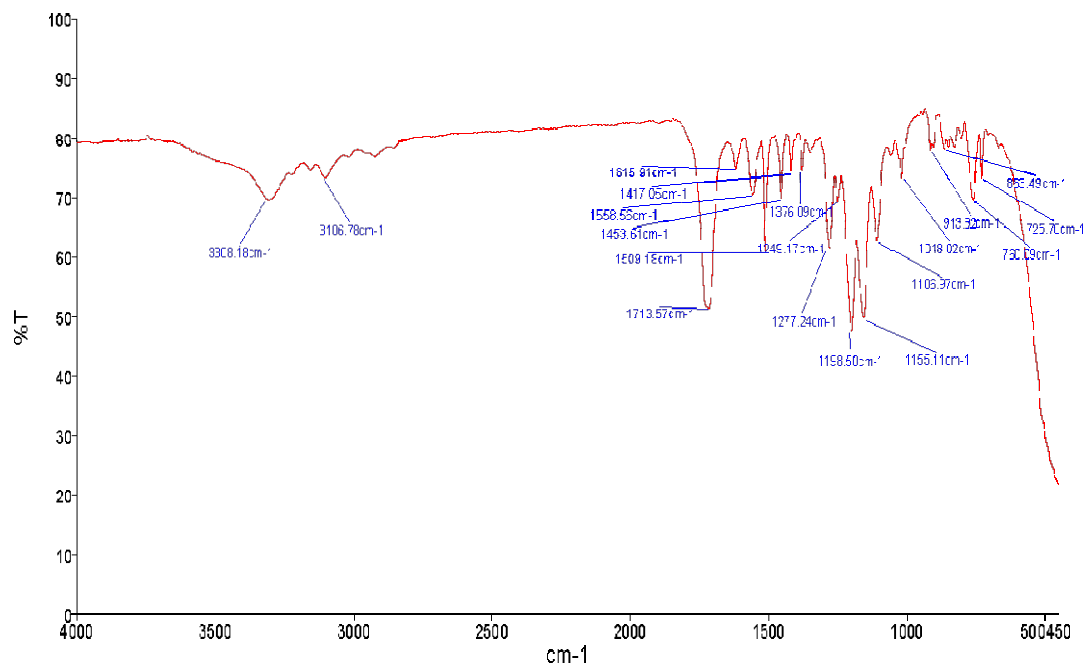


¹H NMR of Compound No. 16

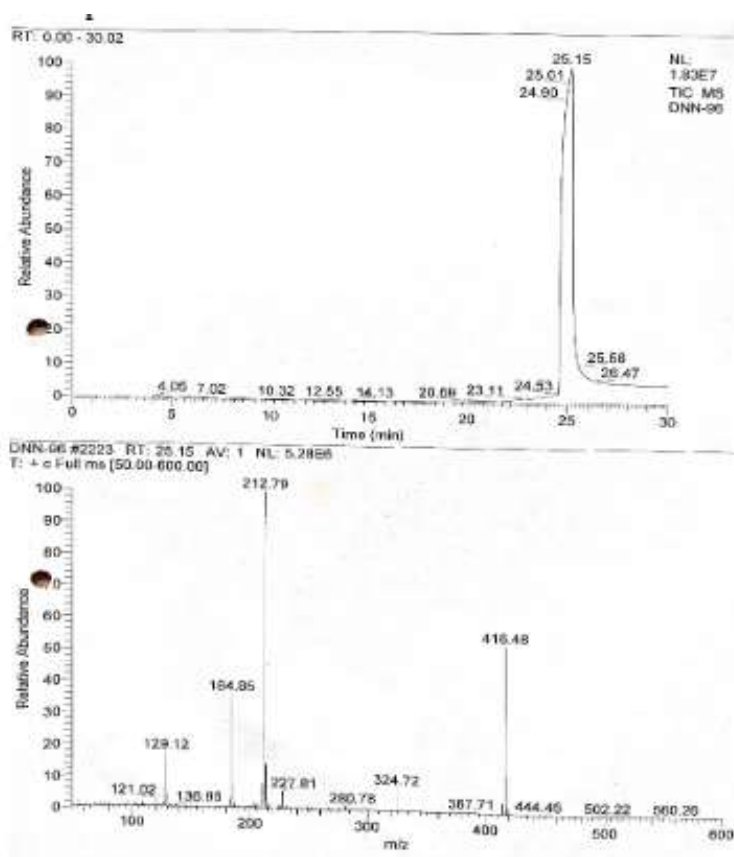


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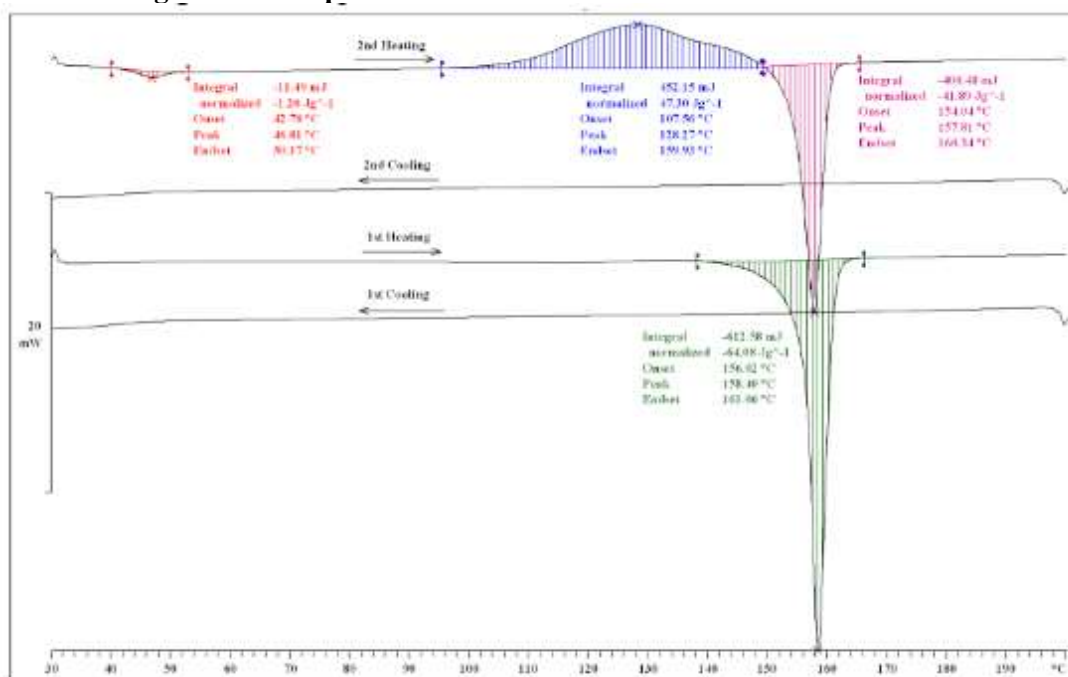
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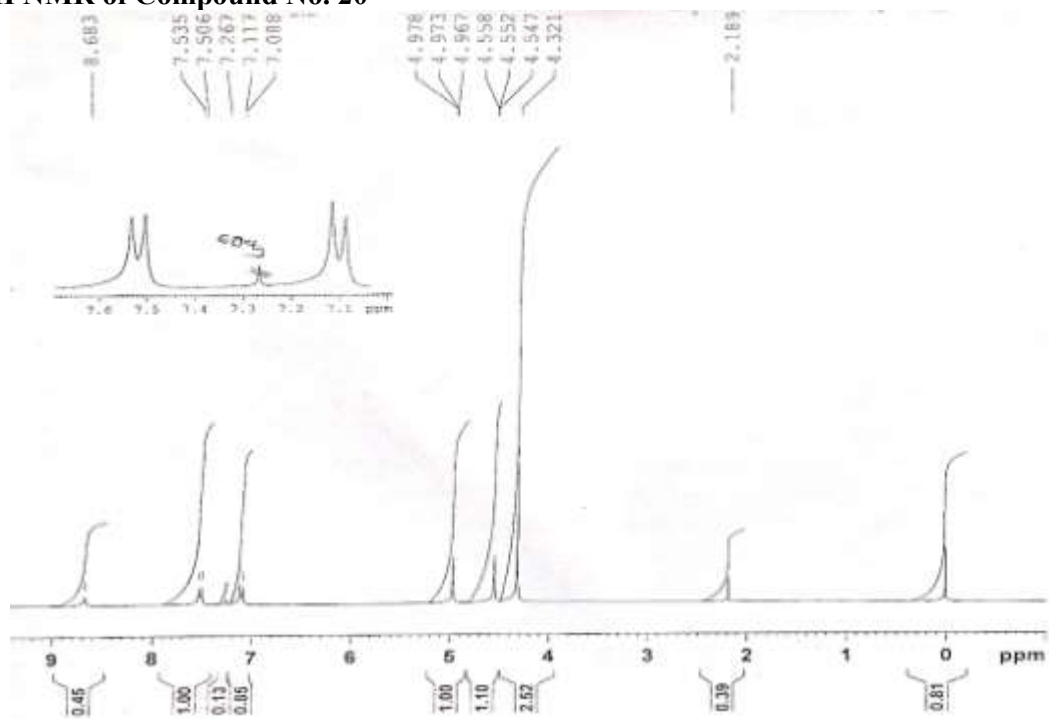
Mass Spectra of Compound No. 20



DSC Thermogram of Compound No. 20

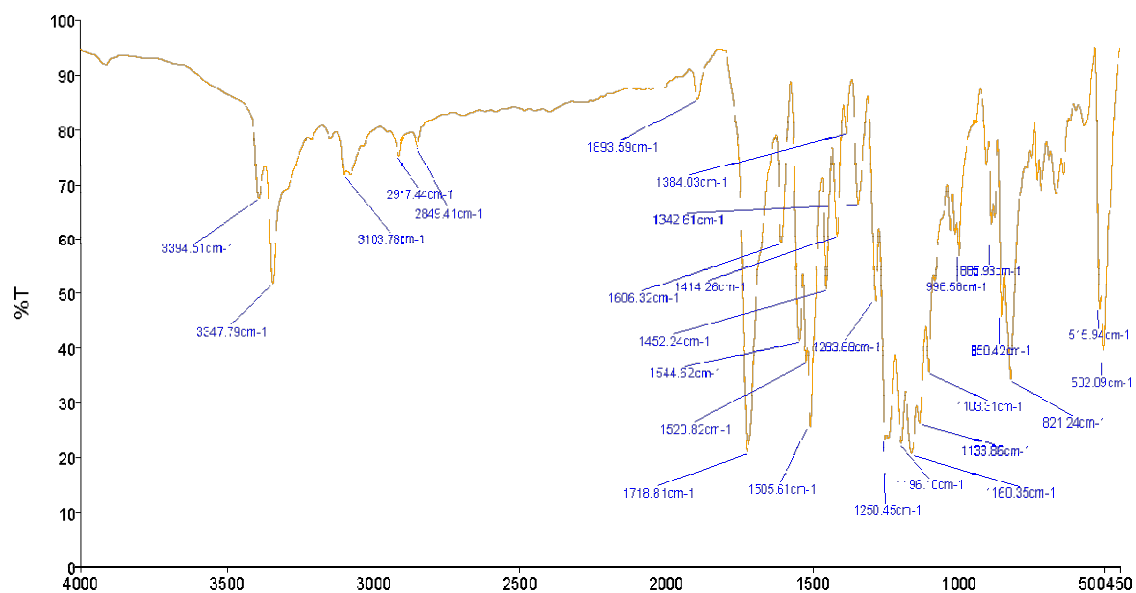


¹H NMR of Compound No. 20

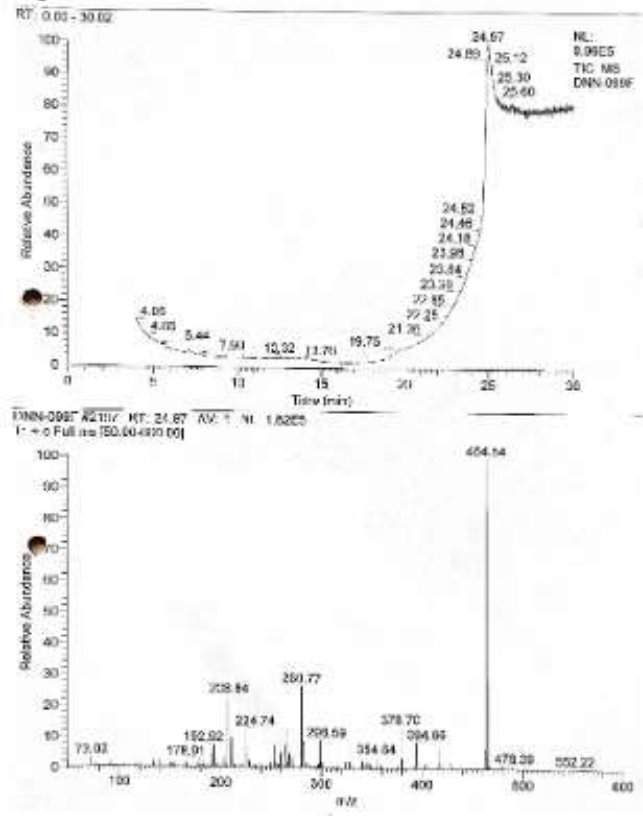


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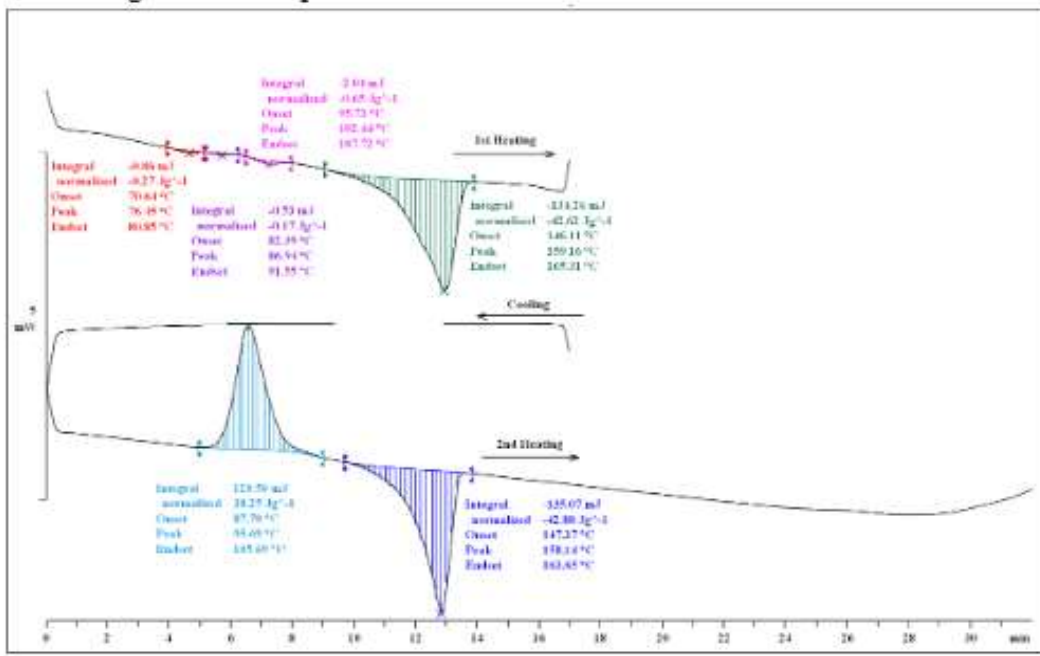
IR Spectra of Compound No. 24



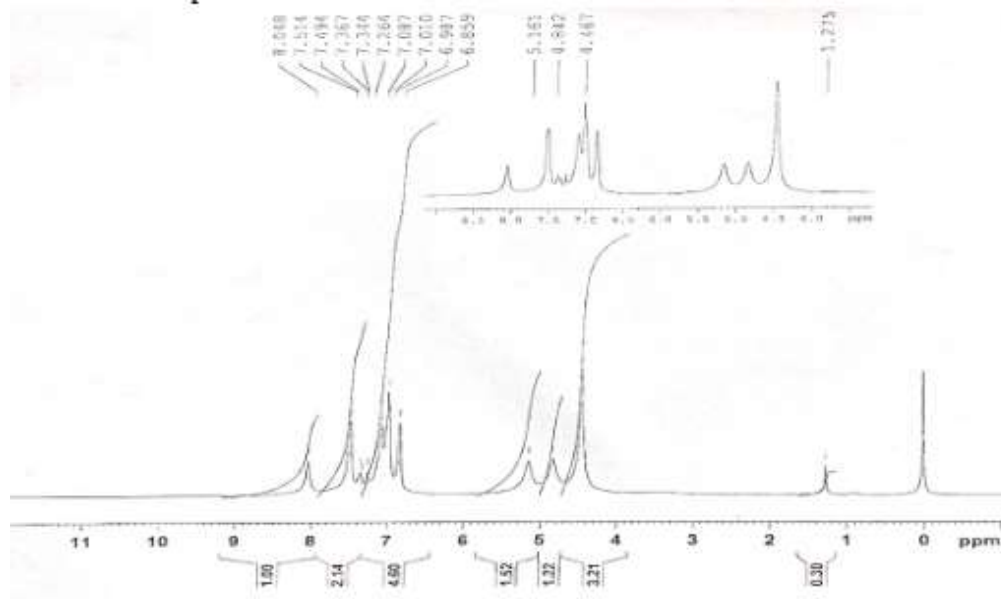
Mass Spectra of Compound No. 24



DSC Thermogram of Compound No. 24

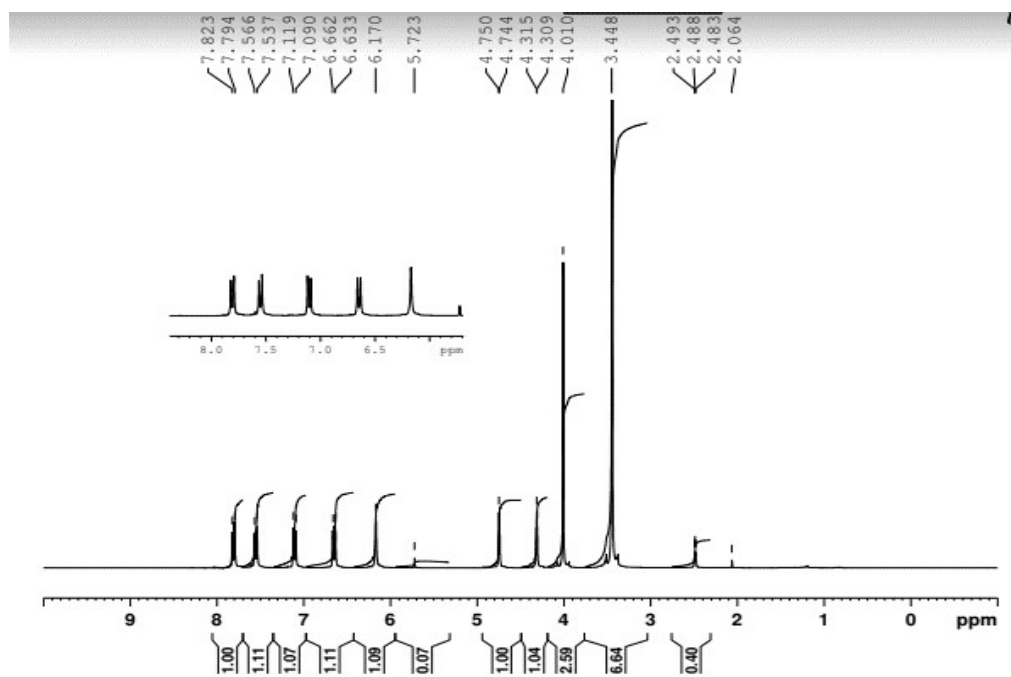


¹H NMR of Compound No. 24



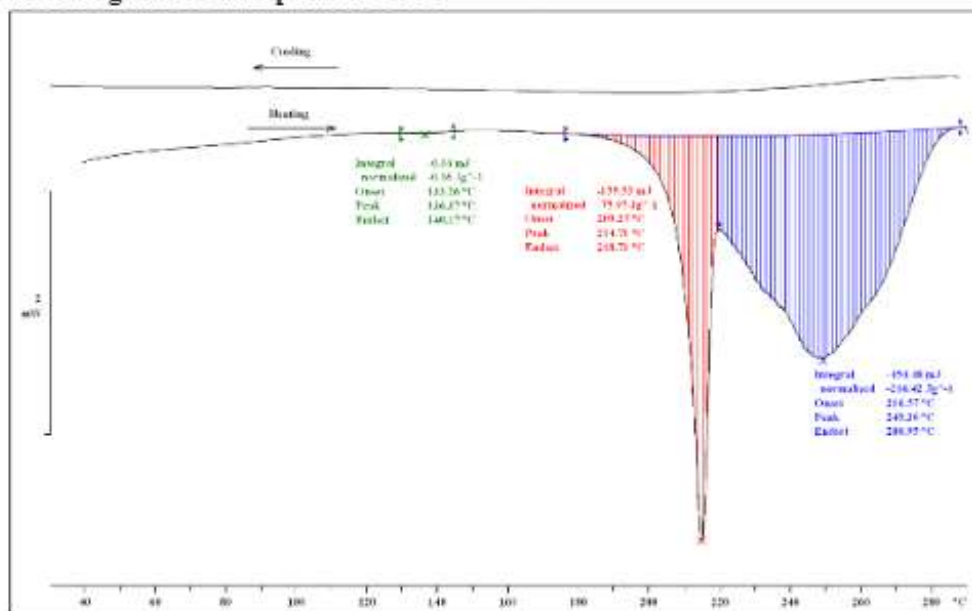
8) Spectral data of Compound No. 27

¹H NMR Spectra of Compound No. 27



9) Spectral data of Compound No. 31

DSC Thermogram of Compound No. 31



¹H NMR Spectra of Compound No. 31

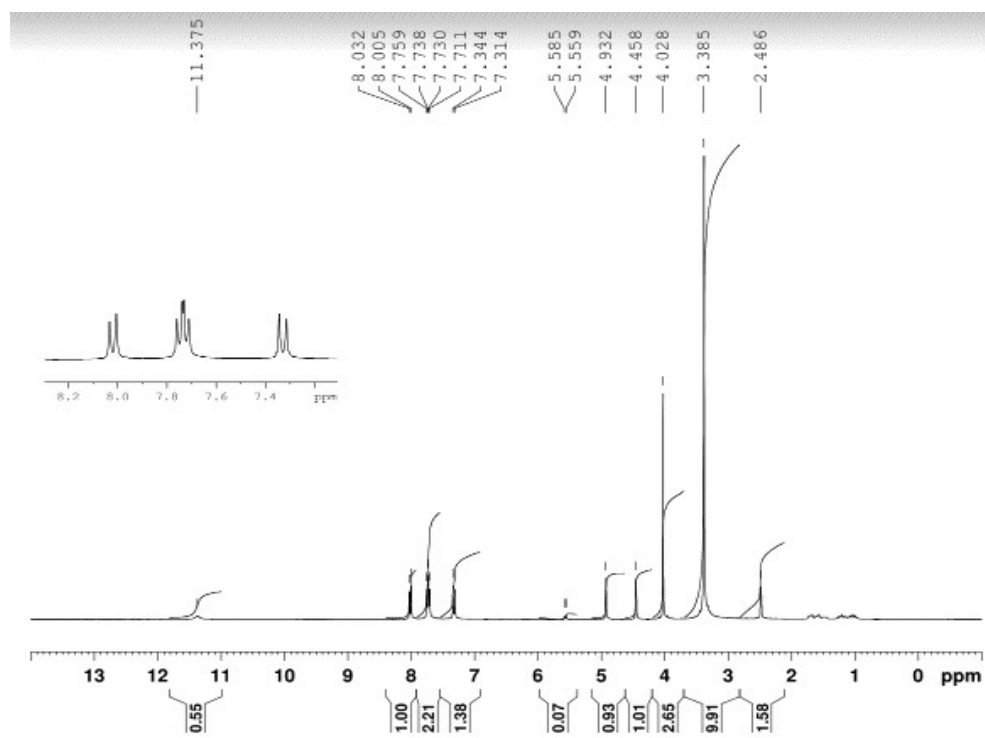
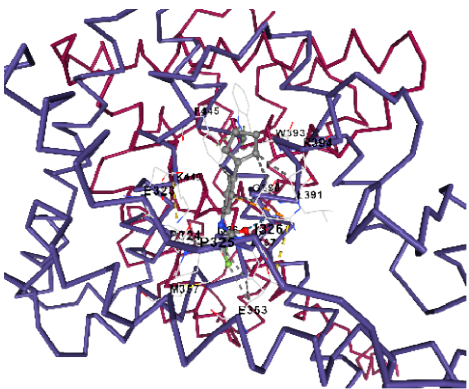
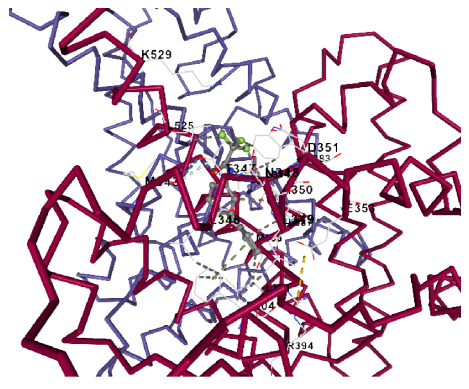
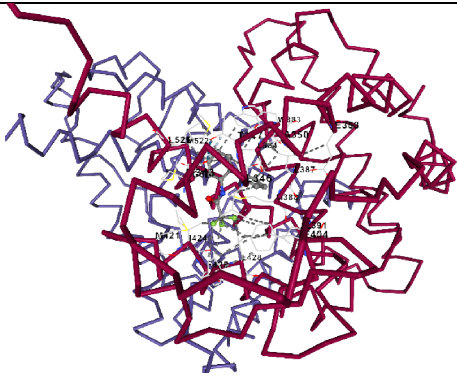
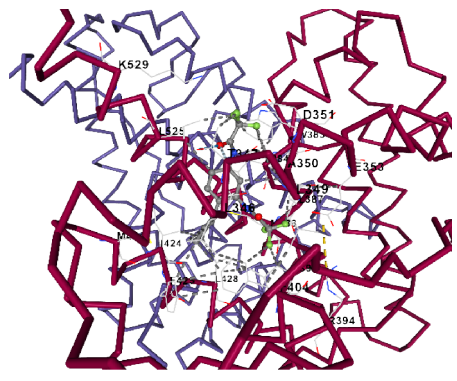
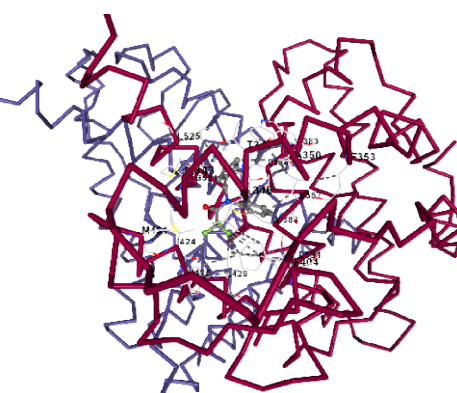
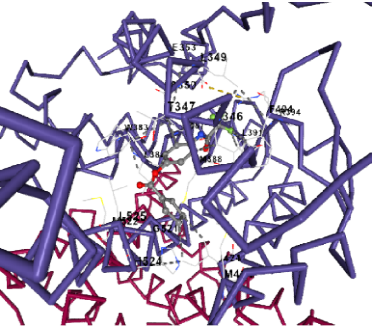
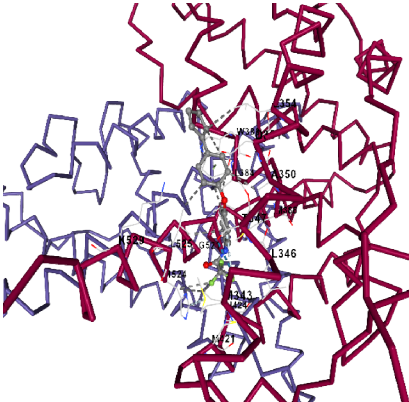
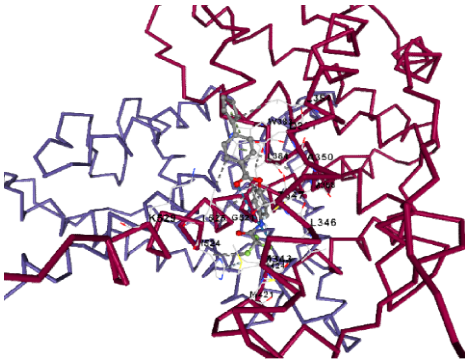


Table 01- Dock score of designed fluorinated ferrocene derivatives

Sr no	Compound	DOCK SCORE	Docking image	Amino acids residues interacting with fluorinated ferrocene derivatives
1		-7.3		GLU323 PRO324 PRO325 ILE326 GLU353 MET357 ILE386 LEU387 GLY390 LEU391 TRP393 ARG394 PHE445 LYS449
2		-8.1		MET343 LEU346 THR347 ASN348 LEU349 ALA350 ASP351 GLU353 TRP383 LEU384 LEU387 MET388 LEU391 ARG394 PHE404 LEU525 LYS529
3		-8.5		MET343 LEU346 THR347 ALA350

				GLU353 TRP383 LEU384 LEU387 MET388 LEU391 PHE404 MET421 ILE424 PHE425 LEU428 GLY521 MET522 LEU525
4		-9.1		LEU346 THR347 LEU349 ALA350 ASP351 GLU353 TRP383 LEU384 LEU387 MET388 LEU391 ARG394 PHE404 MET421 ILE424 PHE425 LEU428 LEU525 LYS529
5		-8.0		MET343 LEU346 THR347 ALA350 GLU353 TRP383 LEU384 LEU387 MET388 LEU391 PHE404 MET421 ILE424 PHE425 LEU428 GLY521 LEU525

6		-8.0		LEU346 THR347 LEU349 ALA350 GLU353 TRP383 LEU384 LEU387 MET388 LEU391 ARG394 PHE404 MET421 ILE424 GLY521 MET522 HIS524 LEU525
7		-8.6		MET343 LEU346 THR347 ALA350 ASP351 LEU354 TRP383 LEU384 MET388 MET421 ILE424 GLY521 HIS524 LEU525 LYS529
8		-9.1		MET343 LEU346 THR347 ALA350 ASP351 LEU354 TRP383 LEU384 MET388 MET421 ILE424 GLY521 HIS524 LEU525 LYS529
9				LEU346

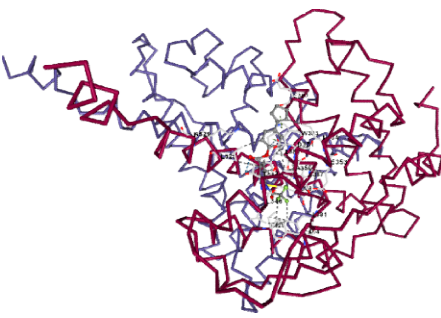
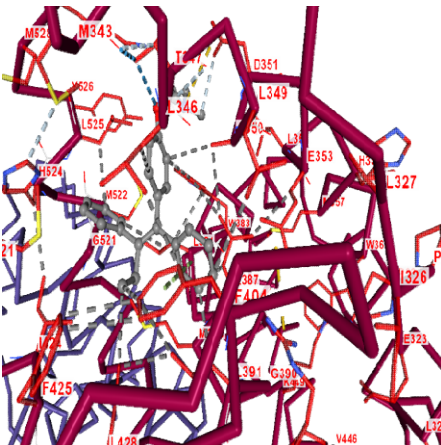
		-9.1		THR347 ALA350 ASP351 GLU353 LEU354 GLU380 TRP383 LEU384 LEU387 MET388 LEU391 PHE404 LEU428 LEU525 LYS529
10	Tamoxifen	-9.1		MET343 LEU346 THR347 LEU349 ALA350 ASP351 GLU353 LEU354 TRP383 LEU384 LEU387 MET388 LEU391 ARG394 PHE404 MET421 ILE424 PHE425 LEU428 GLY521 MET522 HIS524 LEU525 LYS529

Table 02 ADME Properties of fluorinated ferrocene derivatives

Sr NO	Compound No	H-bond Acceptor	H-bond donor	Consensus Log P	ESOL Log S	GI Absorption	BBB	Log Kp	Lipinski
1	04	4	1	3.53	-5.53	High	Yes	-4.68	0
2	07	4	1	3.53	-5.53	High	Yes	-4.68	0
3	10	4	1	3.53	-5.53	High	Yes	-4.68	0
4	13	8	2	3.88	-6.17	Low	No	-5.14	0
5	16	4	0	3.62	-5.69	High	No	-4.61	0
6	20	6	1	3.17	-5.45	High	Yes	-5.18	0
7	24	5	1	4.57	-7.04	Low	No	-4.15	1
8	27	6	1	4.44	-7.06	Low	No	-4.4	1
9	31	6	1	4.44	-7.06	Low	No	-4.4	1
10	Tamoxifen	2	0	5.77	-6.59	Low	No	-3.5	1