

Supporting Information

Planar-Rotor Architecture Based Pyrene-Vinyl-Tetraphenylethylene Conjugated Systems: Photophysical Properties and Aggregation Behavior

Debabrata Jana,^a Shatabdi Boxi,^a Partha P. Parui,^b and Binay K. Ghorai*^a

^a*Department of Chemistry, Indian Institute of Engineering Science and Technology, Shibpur, Howrah 711 103, India*

^b*Department of Chemistry, Jadavpur University, Kolkata 700 032, India*

Tel: +91-33-26684561; Fax: +91-33-26682916; E.mail: binay@chem.iiests.ac.in

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1. Aggregation properties (UV-vis) of 8-10

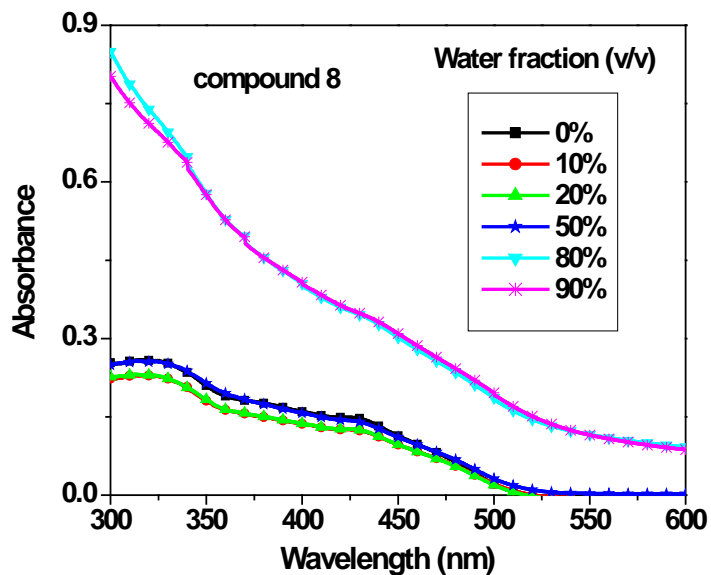


Fig. A Absorption spectra of 8 (10 μ M) in THF and with different amounts of water.

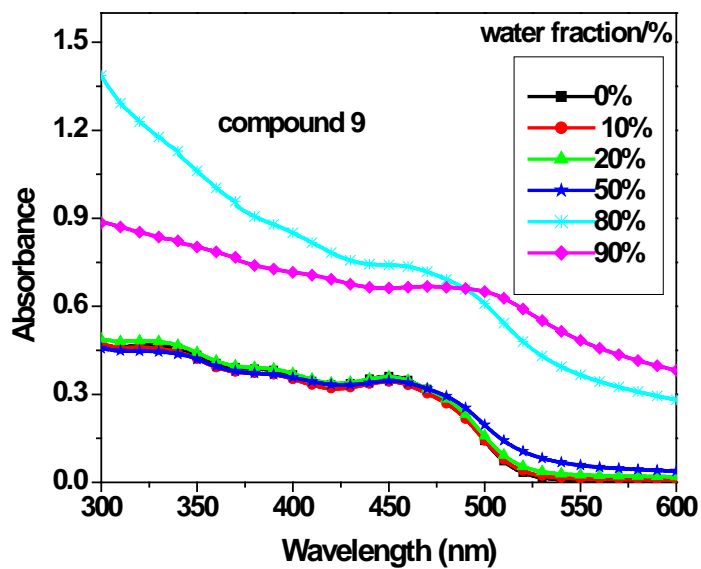


Fig. B Absorption spectra of 9 (10 μ M) in THF and with different amounts of water.

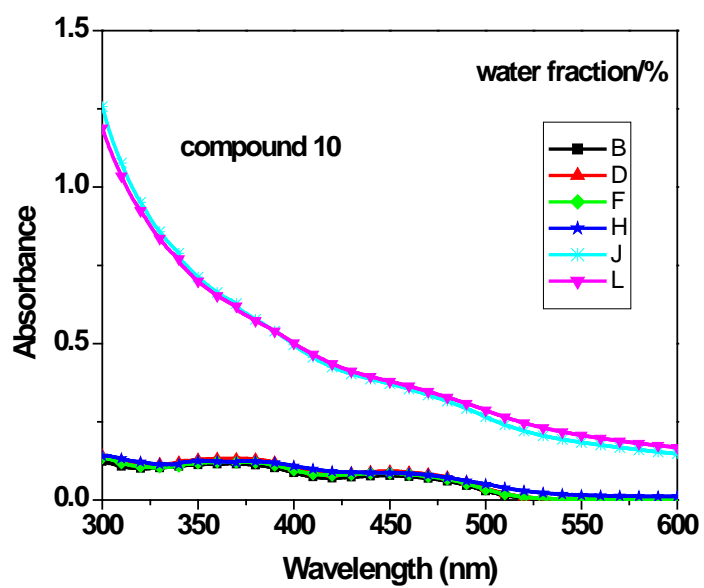


Fig. C Absorption spectra of **10** (10 μM) in THF and with different amounts of water.

2. Theoretical calculation data (HF/6-31G)

For Compound 7:

FOpt[RHF]6-31G|C44H30|PROF. GHORAI

	x	y	z
C,	-5.703826418,	-2.7145876124,	6.1238070431
C,	-4.3387570292,	-2.5214619568,	6.2524474594
C,	-3.5108443648,	-2.5418239624,	5.1313514447
C,	-4.0750491583,	-2.76228533,	3.8553904888
C,	-5.4713378781,	-2.9549402948,	3.7318907758
C,	-6.2663057567,	-2.9286176733,	4.8756989736
C,	-2.0883660466,	-2.3347683309,	5.22366905
C,	-3.2371958236,	-2.7898742988,	2.6920866763
C,	-1.8379663894,	-2.6039354022,	2.8137521333
C,	-1.3017963,	-2.3594500581,	4.1341703817
C,	-1.0282044095,	-2.641148647,	1.6624672647
C,	-1.6322012953,	-2.855666057,	0.4238137295
C,	-2.9971744099,	-3.025442951,	0.3008017097
C,	-3.8205325602,	-3.0010386899,	1.4220088987
C,	-5.246980742,	-3.1924687556,	1.3271318519
C,	-6.0289132701,	-3.1722387965,	2.4189243442
H,	-7.0894158753,	-3.3168893445,	2.3350359241
H,	-5.6716283202,	-3.3536303376,	0.3542297961
H,	-1.6645523116,	-2.1488711658,	6.1925751962
H,	-6.3299337979,	-2.6970179744,	6.9949369441
H,	-3.9087168505,	-2.3531115376,	7.221782685
H,	-7.3258863399,	-3.0757042525,	4.7832244083
H,	-0.252320998,	-2.1766961768,	4.2408616096
H,	-1.0148024639,	-2.9189688846,	-0.4505160159
H,	-3.4279994442,	-3.1949715712,	-0.6679994743
C,	0.4388991526,	-2.4852919136,	1.7473483977
C,	1.1823337638,	-1.8185393097,	0.8650890634

H,	0.9184955711,	-2.9531171447,	2.586860967
H,	0.688437946,	-1.2949257978,	0.0650654311
C,	2.6488359789,	-1.6773239677,	0.885904182
C,	3.243250421,	-0.6423621435,	0.1656243739
C,	3.4887764058,	-2.5447928003,	1.5881936647
C,	4.6159843269,	-0.457719218,	0.169614685
H,	2.6249479963,	0.0305144127,	-0.3987052163
C,	4.8596127183,	-2.3656428776,	1.5849576022
H,	3.0747842106,	-3.3784924064,	2.1210054393
C,	5.4497589468,	-1.3089701403,	0.8892728836
H,	5.0411098701,	0.3536221532,	-0.387211442
H,	5.4817433191,	-3.0586620385,	2.1180032892
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C,	9.6320118598,	0.04774404,	-0.2330820175
C,	9.8107109395,	0.6708910 281,	2.0730362212
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H,	11.7569877973,	1.2302898191,	2.7419689803
H,	12.8114294788,	0.889630129,	0.5385950523
C,	6.826199124,	1.1867414259,	1.7716122473
C,	6.9426224936,	2.4438258578,	1.1775002186
C,	6.0630393236,	1.069681808,	2.9315528987
C,	6.2928389839,	3.5451978434,	1.7118717902
H,	7.5455007916,	2.5578238751,	0.2970103085
C,	5.4199955684,	2.1731931538,	3.473284961
H,	5.9701953549,	0.113460919,	3.4075667105

C,	5.5283374418,	3.4135649885,	2.8629764734
H,	6.3866736274,	4.5020426163,	1.2348594135
H,	4.8376828098,	2.0625838286,	4.3679308878
H,	5.0289674619,	4.2667794644,	3.2803086001
C,	7.6873970962,	-2.3840004993,	0.4762293634
C,	7.3769470182,	-3.0387996873,	-0.7160680026
C,	8.6671765059,	-2.9348717776,	1.2995947046
C,	8.0450183904,	-4.1951563726,	-1.0865665033
H,	6.6091049666,	-2.641637781,	-1.3520454052
C,	9.330109428,	-4.0977618151,	0.9348119638
H,	8.9128903667,	-2.4505011692,	2.2239754874
C,	9.0250087664,	-4.7293798717,	-0.2612881837
H,	7.7985806878,	-4.6792025286,	-2.0122391194
H,	10.0808171519,	-4.5069429792,	1.5834575426
H,	9.5390522094,	-5.6277050748,	-0.5446989759

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[X(C44H30)]

For Compound 8/9:

FOpt[RHF|6-31G|C128H90|PROF. GHORAI|23-Nov-2014

	x	y	z
C,	0.3766651327,	-3.627646068,	0.4609951251
C,	-0.8824898107,	-3.0452739545,	0.4782095061
C,	-0.9827067989,	-1.6462607768,	0.3640112209
C,	0.1969041076,	-0.8729169,	0.1999367148
C,	1.4668958766,	-1.5062739418,	0.1522530534
C,	1.546388782,	-2.9049660995,	0.2689418603
C,	-2.2413265667,	-0.9541497128,	0.4627912874
C,	0.1044131732,	0.5634342233,	0.0803942327
C,	-1.1642104982,	1.1920598789,	0.0947187364
C,	-2.3272108909,	0.3788979352,	0.3295519665
C,	-1.2570777212,	2.5851367248,	-0.080445926
C,	-0.0883416916,	3.3186674315,	-0.2119155019
C,	1.1763232638,	2.7435762473,	-0.1562315301
C,	1.2835690726,	1.3466166988,	-0.0457283297
C,	2.5494043766,	0.6607944724,	-0.0829013531
C,	2.6351801151,	-0.6748677337,	0.0143322742
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H,	3.4416923108,	1.2369579389,	-0.2013972026
H,	-3.1224468491,	-1.5213246684,	0.6737570038
H,	0.4468639094,	-4.6954352006,	0.5568115968
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H,	-0.1604443595,	4.3781436213,	-0.3657957767
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H,	3.5595296694,	-2.9281543041,	-1.5851296969
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C,	5.5753440028,	-4.5566827727,	-2.1093097261

C,	5.5307467921,	-5.0609924835,	0.2247640971
C,	6.7229729667,	-5.3162894231,	-2.2540425379
H,	5.1585020767,	-4.0638635812,	-2.9677865843
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H,	5.1053673095,	-4.9447319767,	1.2023928526
C,	7.2839740286,	-5.9821571657,	-1.1655915586
H,	7.1882877724,	-5.3912328609,	-3.2179824011
H,	7.0963085506,	-6.3109030965,	0.9365638943
C,	8.5405157554,	-6.7830896108,	-1.3279260272
C,	8.6529035031,	-8.0595017047,	-0.9187931503
C,	9.9558234815,	-8.8031632797,	-0.9128120944
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H,	11.3180438525,	-11.6939060326,	-2.0356078557
H,	13.1056680948,	-8.6200519755,	0.3145507225
H,	13.2795068036,	-10.7885765737,	-0.8457011127
C,	7.4860805197,	-8.865930233,	-0.4299391435
C,	7.5443271709,	-9.508887678,	0.8070440786
C,	6.3446205649,	-9.0337240887,	-1.2113136958
C,	6.4817521387,	-10.2742613401,	1.2607777888
H,	8.4251126694,	-9.4104311197,	1.4122166754
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H,	11.4050026826,	-3.1470132045,	-1.6969396119
H,	11.7597256683,	-6.209667516,	-4.6400629926
H,	12.4959892515,	-4.044618509,	-3.7185850887
C,	-2.0394489725,	-3.963076923,	0.6090653246
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C,	-6.3655920193,	-10.3381961985,	-2.3984314872
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C,	-7.4626269399,	-10.4754788922,	-3.2378185386
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H,	-9.447197214,	-9.8035497832,	-3.6588304563
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C,	-8.6981008645,	-6.9171894873,	3.3711792953
C,	-8.7771515727,	-5.2683462616,	1.6351934057
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H,	-8.6265125555,	-7.942729547,	3.6791494939
C,	-8.9283506483,	-4.2721081912,	2.5888438351
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H,	-9.0251019302,	-3.2495029956,	2.2779149343
H,	-9.0693497189,	-3.8238935972,	4.6751809376
C,	2.3302762354,	3.6709471167,	-0.2412939779
C,	3.3755484044,	3.7041947075,	0.5829243212
H,	2.2426655438,	4.4239763137,	-1.0053682905
H,	3.4165931246,	3.0015390267,	1.3965994651

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C,	5.2763672276,	4.8596940578,	1.6690160214
C,	4.8333439633,	5.3759030067,	-0.6203534623
C,	6.3324214409,	5.7539773536,	1.6689310191
H,	5.0511509956,	4.3112134642,	2.5646112654
C,	5.8823473208,	6.2784382501,	-0.6169472748
H,	4.2880789407,	5.2170635524,	-1.5301047634
C,	6.6450721079,	6.4940745473,	0.5299234064
H,	6.9199826002,	.8769815034,	2.5583049238
H,	6.1161732211,	6.8163255761,	-1.514293239
C,	7.805660711,	7.4426163101,	0.532741805
C,	7.7025570291,	8.7266608352,	0.1456033078
C,	8.8913250112,	9.6254923339,	-0.0264535544
C,	8.937771627,	10.861156274,	0.6199660834
C,	9.9470403543,	9.2764782034,	-0.8661617791
C,	10.020167307,	11.7103409877,	0.4528250429
H,	8.1227748661,	11.1570887777,	1.2523414456
C,	11.0266834186,	10.1298072596,	-1.0423225115
H,	9.9245195659,	8.3351206836,	-1.37875429
C,	11.0696231484,	11.3472598586,	-0.3800655019
H,	10.0419492789,	12.6526059763,	0.9662302353
H,	11.8292586435,	9.8431664102,	-1.6945976862
H,	11.9055957327,	12.0065636469,	-0.514416508
C,	6.3884325693,	9.3870834065,	-0.1505162342
C,	6.1885935895,	10.0423445661,	-1.366074813
C,	5.3604761743,	9.4064231932,	0.7899902053
C,	4.9867684936,	10.6743442535,	-1.6434510468
H,	6.9777098527,	10.0581769107,	-2.0932362983
C,	4.1604191209,	10.047182048,	0.5177549288
H,	5.4994066499,	8.9166211302,	1.7335498037
C,	3.9672882839,	10.6790368805,	-0.7013424089
H,	4.8486532615,	11.164762508,	-2.5880843747

H,	3.3814983546,	10.0519934562,	1.2559895805
H,	3.0383665829,	11.1728371734,	-0.9130734713
C,	9.092870518,	6.8346004908,	1.0068743462
C,	9.5754765894,	5.6639071353,	0.4208990105
C,	9.8077389351,	7.3891957039,	2.0664300788
C,	10.7519090571,	5.0803023334,	0.863694501
H,	9.0260491193,	5.2098084539,	-0.3814207418
C,	10.9804673963,	6.8007355531,	2.5173949381
H,	9.4474329233,	8.2836303752,	2.5350777322
C,	11.4592645022,	5.647311338,	1.9149313991
H,	11.1119998425,	4.1850986005,	0.3937287012
H,	11.5158277311,	7.2426548549,	3.3358305059
H,	12.3674393958,	5.1931347686,	2.2620921573
C,	-2.5665835632,	3.2675935146,	-0.1435797572
C,	-2.8289645735,	4.4570599723,	0.3968292745
H,	-3.3457866025,	2.7492069201,	-0.6709392822
H,	-2.0654741927,	4.9375518072,	0.98363345
C,	-4.1031001759,	5.192496867,	0.3131458782
C,	-4.3750746072,	6.1924377343,	1.2476803032
C,	-5.0605685574,	4.9484764586,	-0.67224273
C,	-5.5618082537,	6.9032772873,	1.2141146363
H,	-3.6508098736,	6.4130305542,	2.0095340481
C,	-6.2523274709,	5.6512591103,	-0.6986424966
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C,	-6.5316616705,	6.6341050226,	0.249836496
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C,	-9.0211154642,	6.8547641353,	0.1822899571
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C,	-10.4470248868,	8.4360546293,	-1.170451214

C,	-12.5250633921,	8.2236627466,	0.6476434389
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C,	-11.6310450837,	9.1266002937,	-1.3851142183
H,	-9.645607454,	8.5227385859,	-1.8772963904
C,	-12.6722656083,	9.026894941,	-0.4748740663
H,	-13.3269264121,	8.1363642687,	1.3556779422
H,	-11.7376764745,	9.7387506155,	-2.2601272313
H,	-13.5873966683,	9.5626242527,	-0.6395067506
C,	-9.2368152197,	5.3832952708,	0.3797431996
C,	-9.9683576921,	4.6481444361,	-0.5536955893
C,	-8.7602423716,	4.7280574887,	1.5134060022
C,	-10.1931113729,	3.2926807731,	-0.3722398047
H,	-10.3634859253,	5.1409725812,	-1.4212701198
C,	-8.9928125647,	3.3732957421,	1.7014123473
H,	-8.2044167799,	5.2786355027,	2.2464813014
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H,	-10.7501811813,	2.7423781135,	-1.1062450041
H,	-8.6185170254,	2.8874844398,	2.5821174667
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C,	-6.7676365307,	9.501138808,	-0.7565747775
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C,	-6.5541301877,	10.8704503552,	-0.7647131304
H,	-6.2858991746,	8.8836998238,	-1.4903968509
C,	-7.9700015465,	11.1004923314,	1.1560422726
H,	-8.8259865198,	9.2949997619,	1.90235568
C,	-7.1551842781,	11.6758510594,	0.1929022054
H,	-5.9183223364,	11.3058371484,	-1.5117831614
H,	-8.4332450611,	11.7134404569,	1.9053335144
H,	-6.9862224657,	12.7355784221,	0.1906728802

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For Compound 10:

FOpt[RHF|6-31G|C152H106|PROF. GHORAI

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C,	-19.6440760269,	-28.7346205559,	-25.0276150457
C,	-19.2173603851,	-29.9075618492,	-25.6744164571
C,	-17.456573611,	-28.7479281148,	-21.9671243961
C,	-19.4931738326,	-27.1687539872,	-23.1117907167
C,	-18.9359447139,	-26.8241291506,	-21.8566404192
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H,	-16.6401082523,	-29.3094857146,	-21.566390705
H,	-17.8843286247,	-31.5552870846,	-25.5959066848
H,	-17.3814158594,	-27.3354566255,	-20.4328143816
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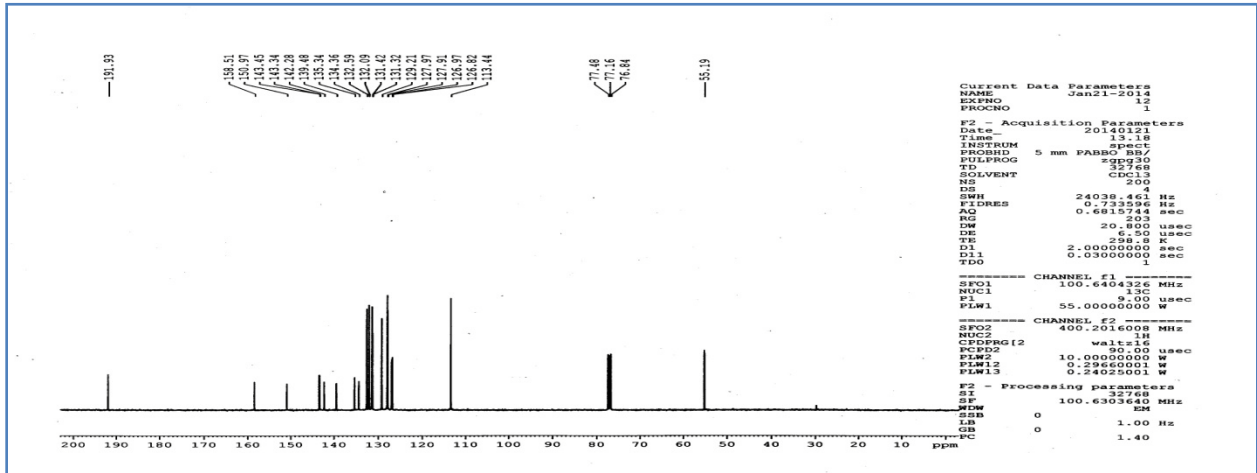
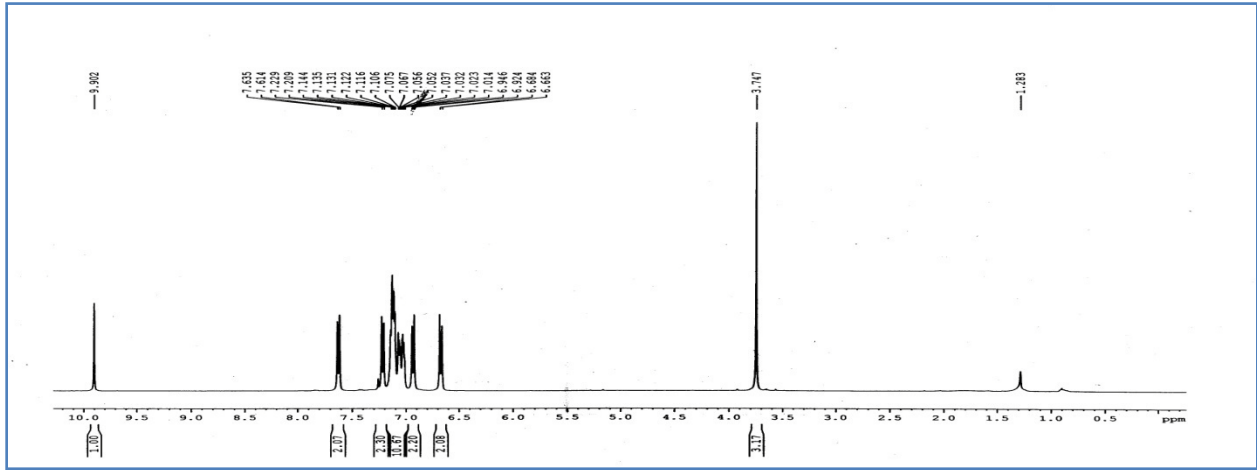
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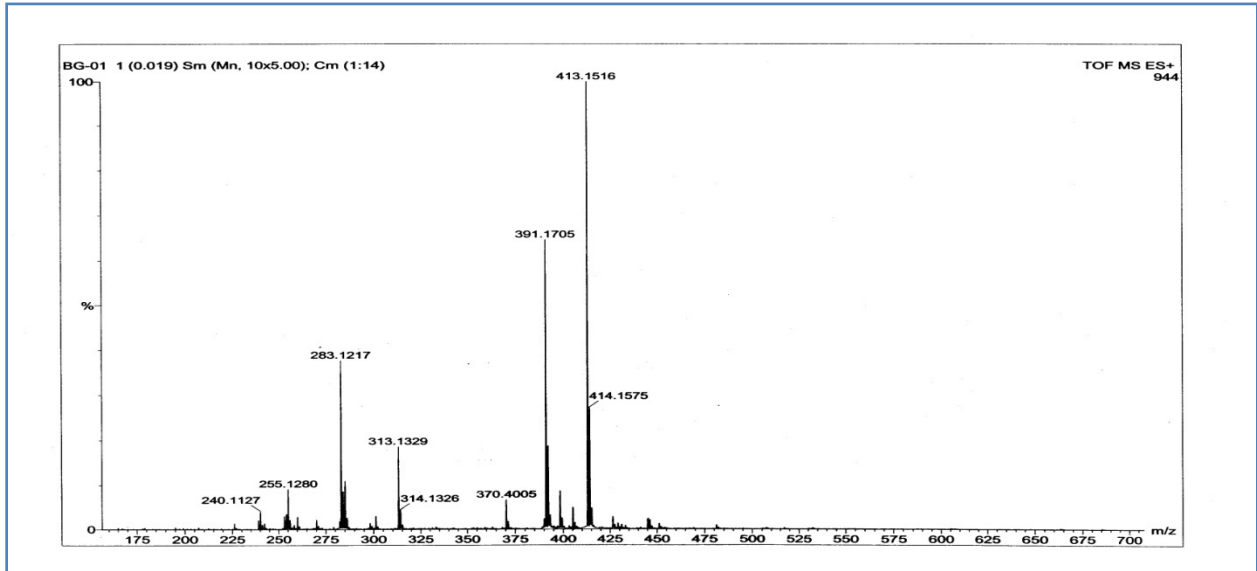
3. Copies of NMR and Mass spectroscopy

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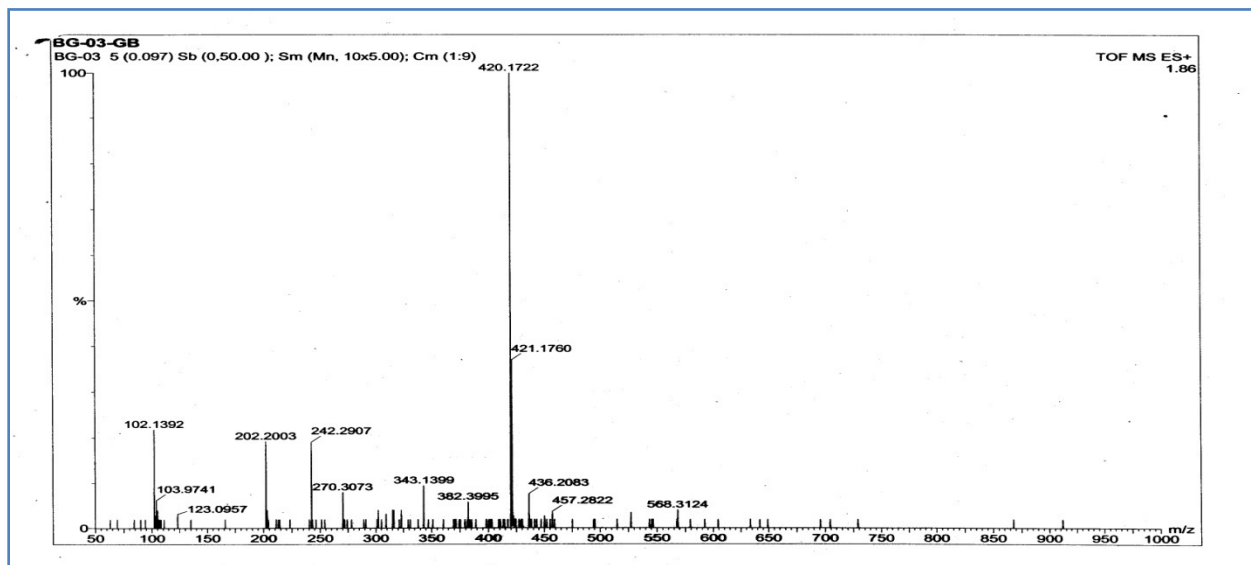
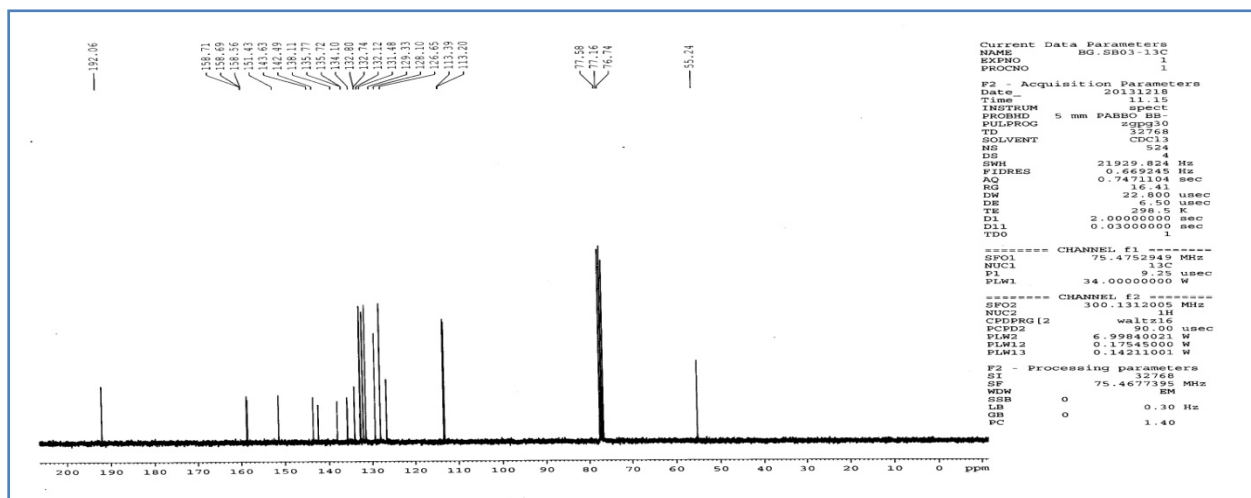
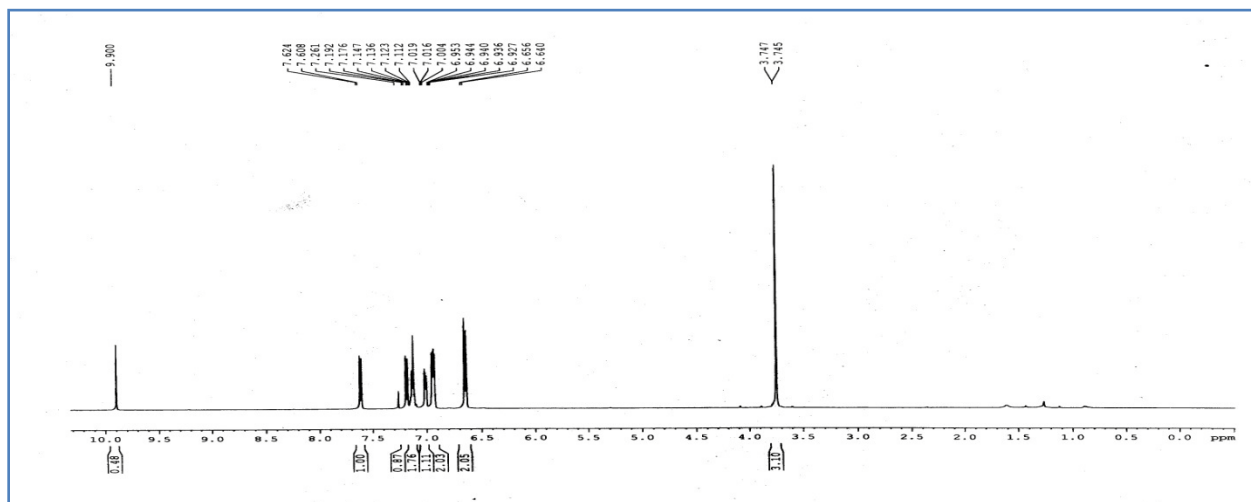


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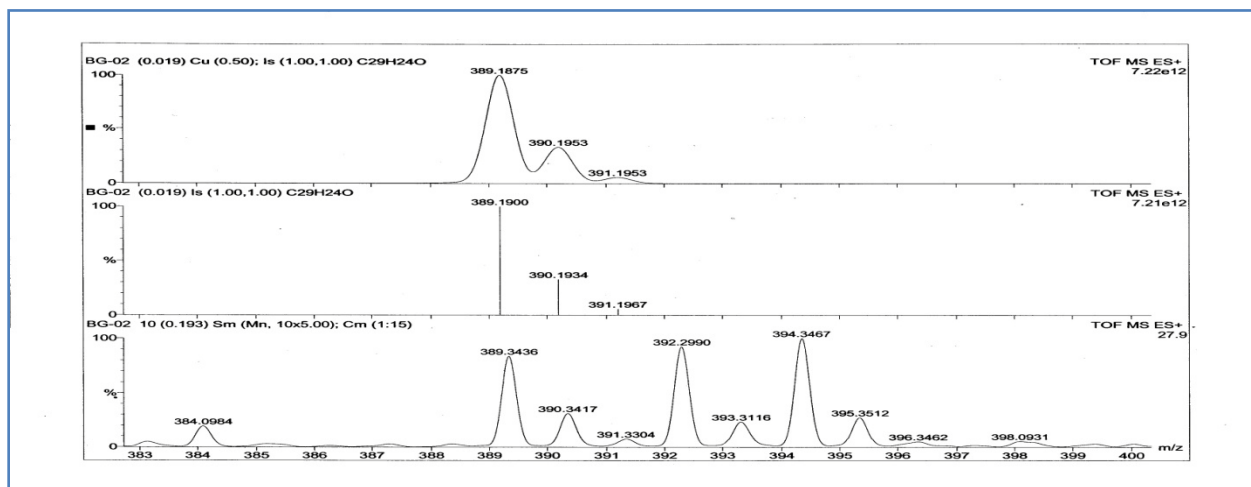
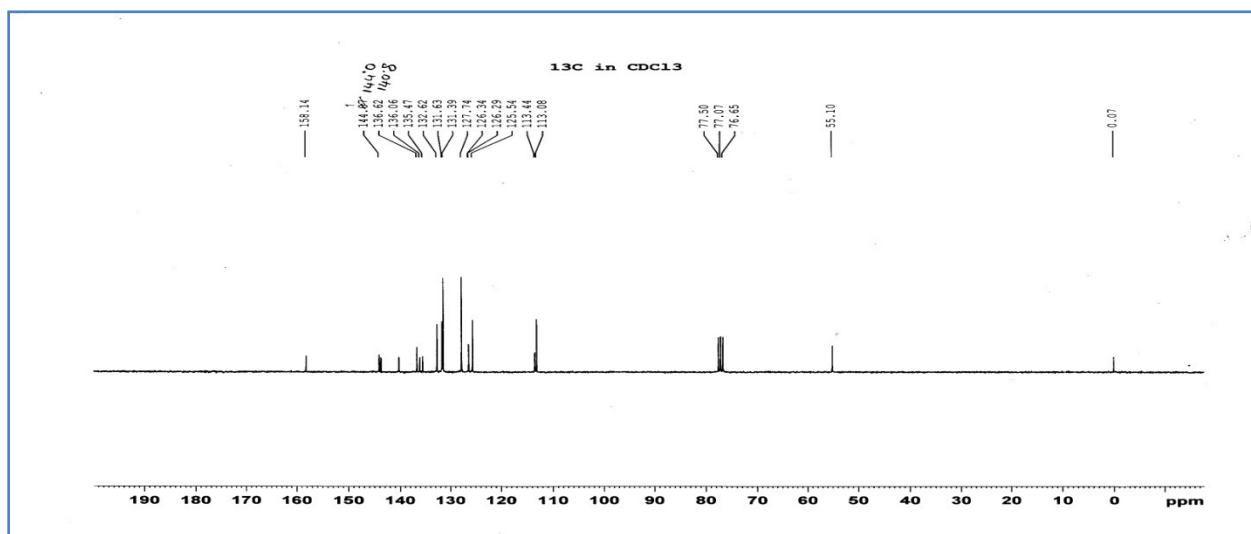
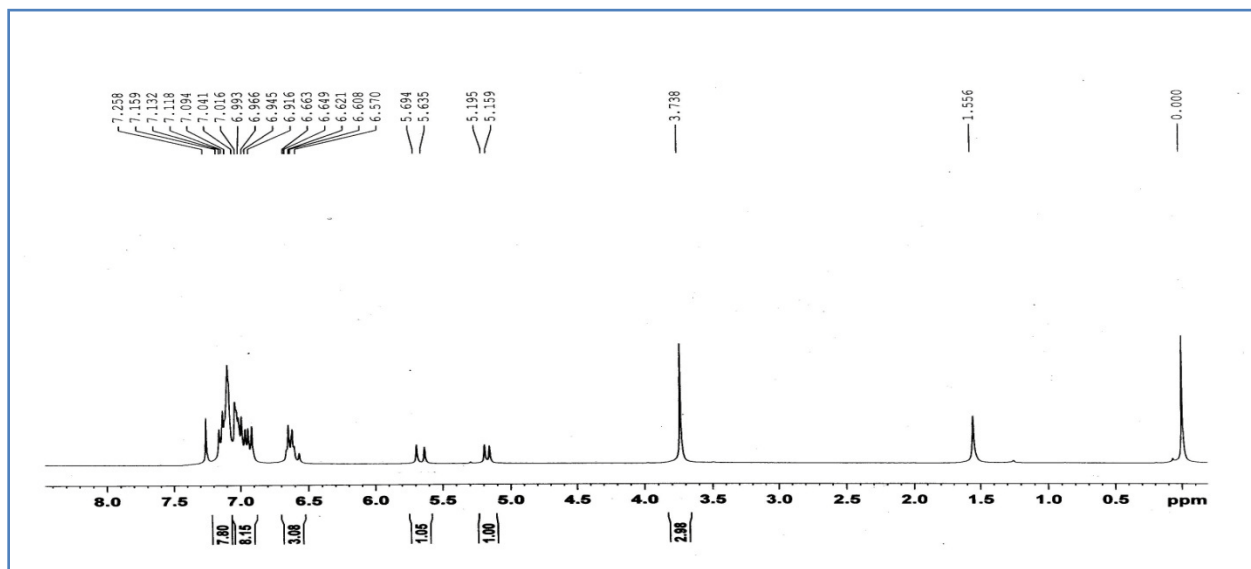
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TD        32768
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SWH       24038.461 Hz
FIDRES    0.733596 Hz
AQ         0.6915744 sec
RG         203
DM         20.800 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TDO        1
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SFO1      100.626125 MHz
NUC1       13C
SI         9.00 usec
PLW1       55.00000000 W
----- CHANNEL f2 -----
SFO2      400.2016008 MHz
NUC2       1H
CPDPRG2   waltz16
PCPD2      80.00 usec
PLW2       10.00000000 W
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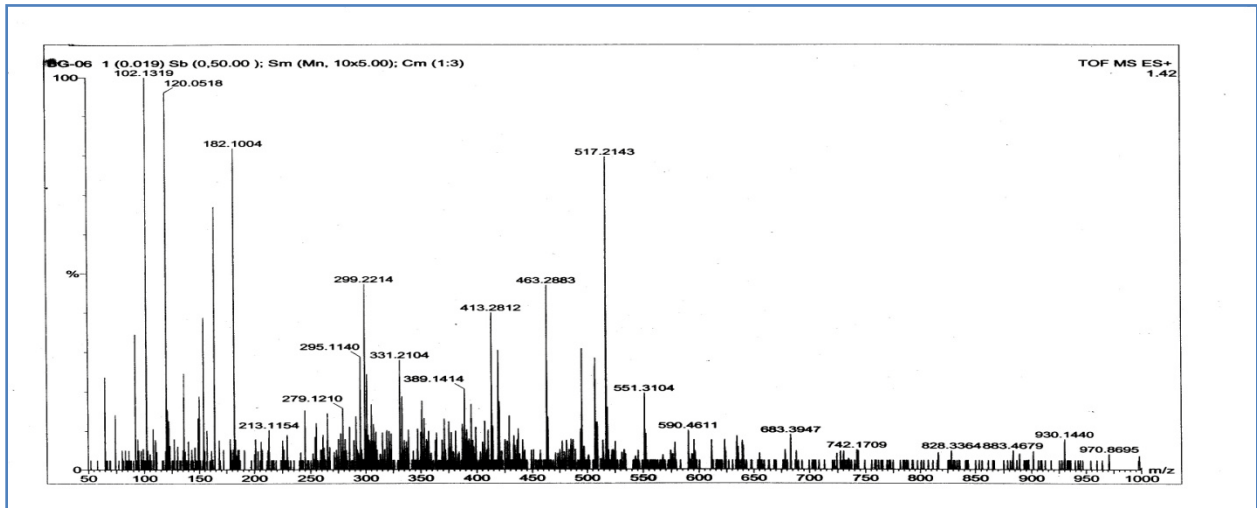
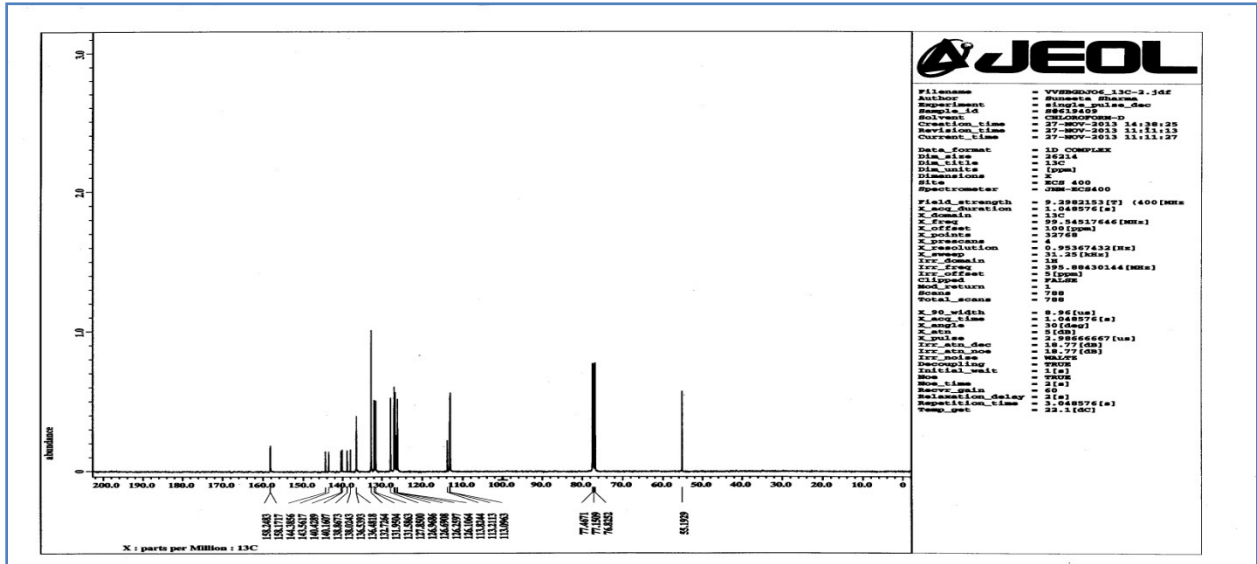
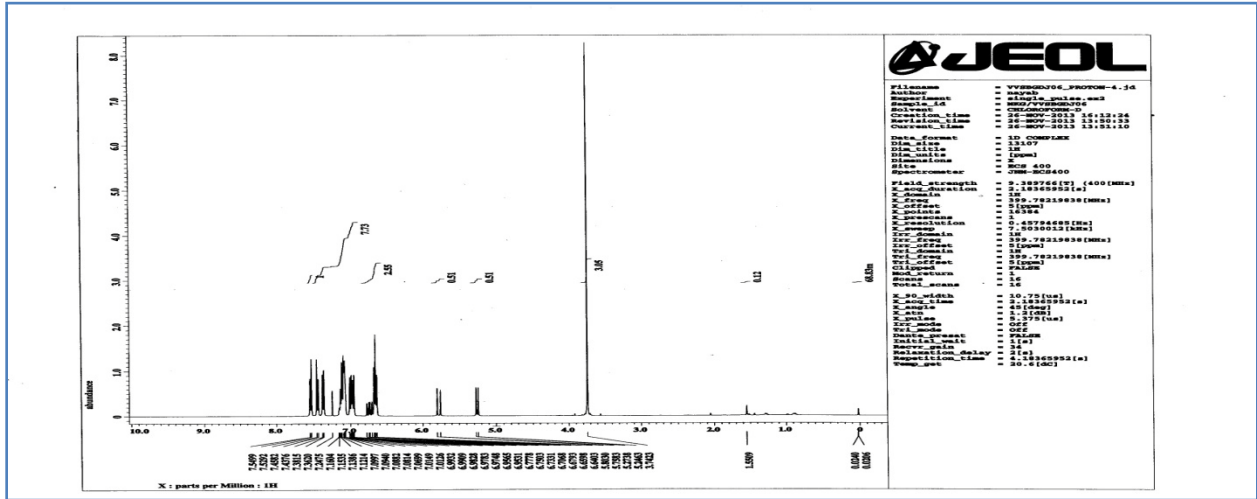
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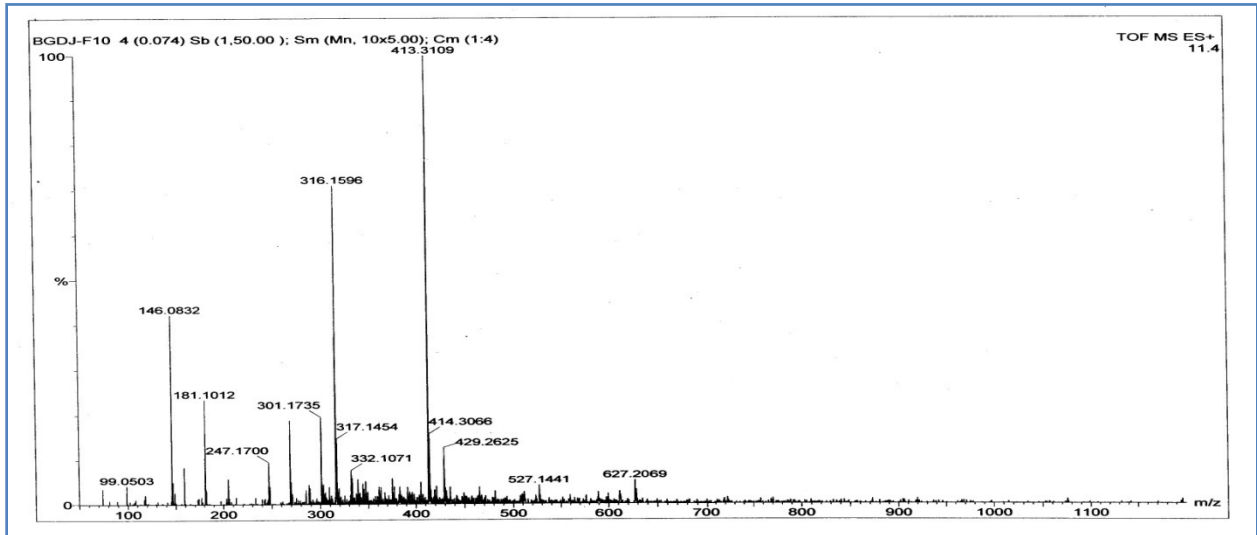
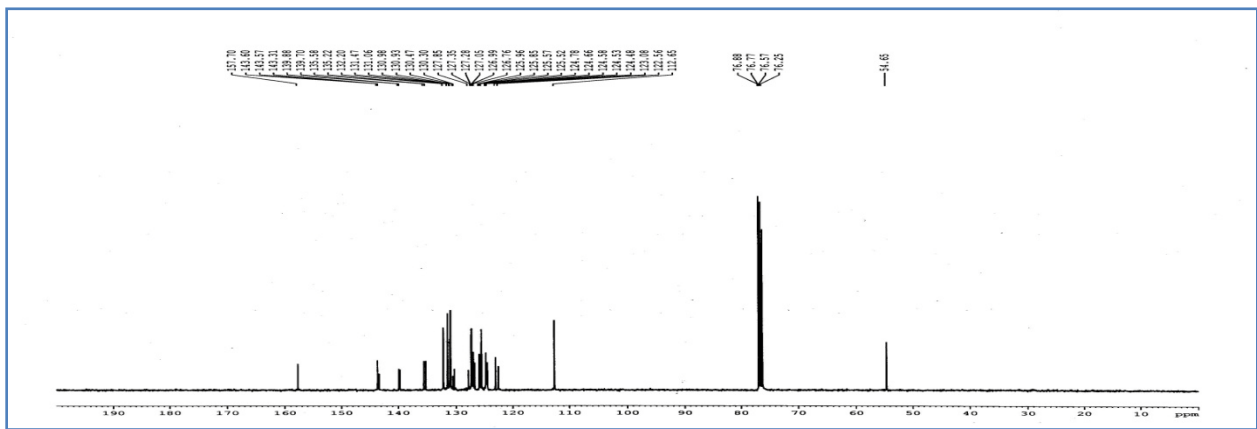
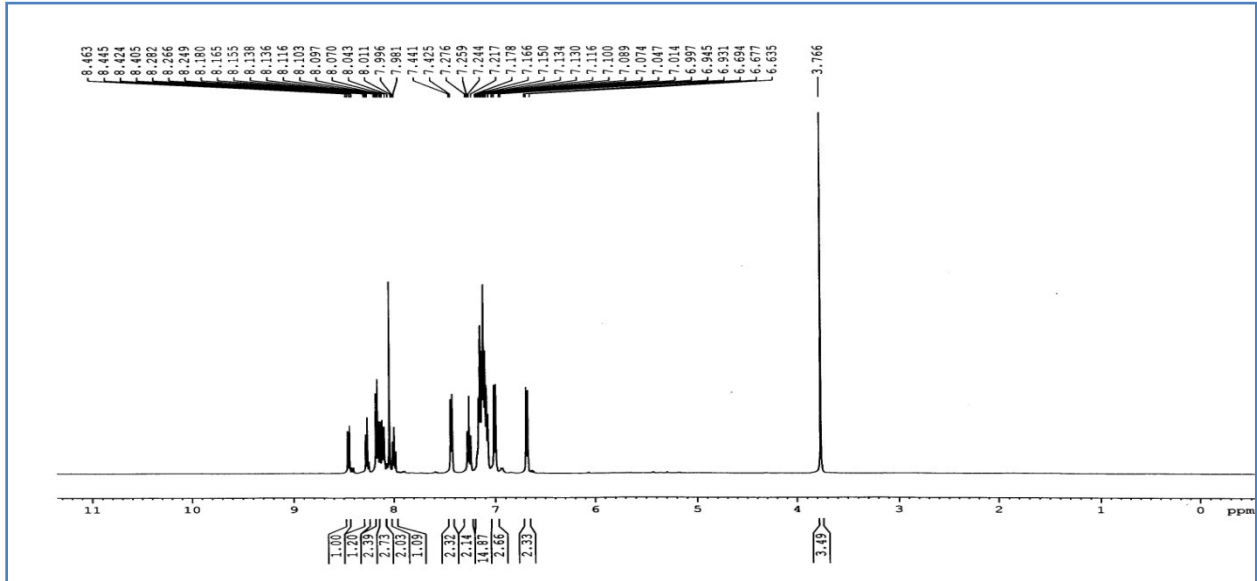
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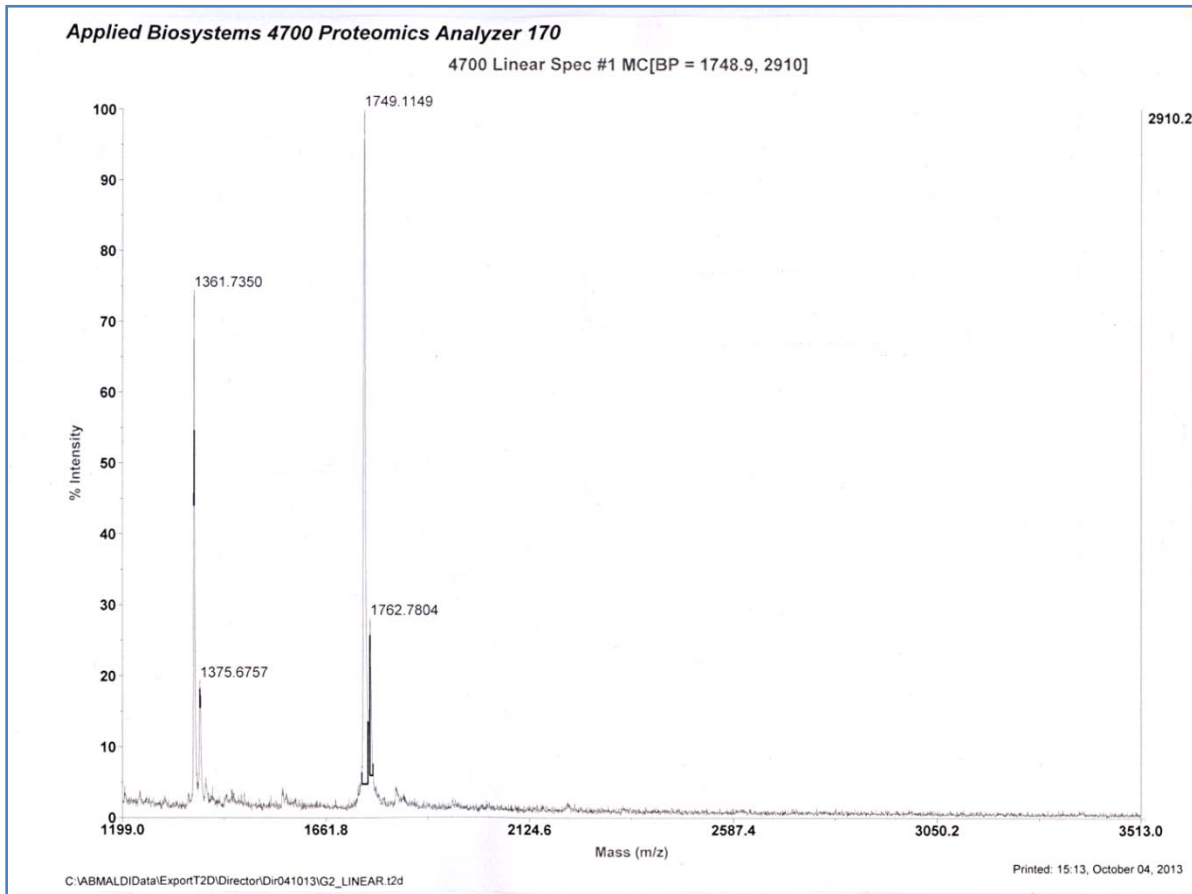
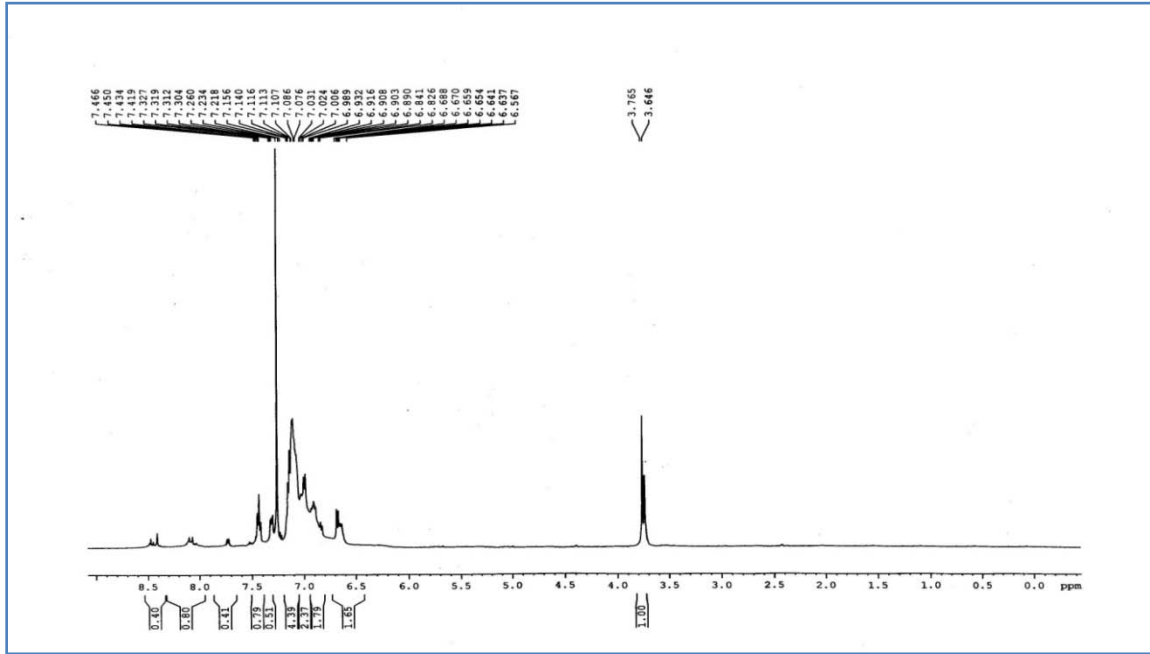
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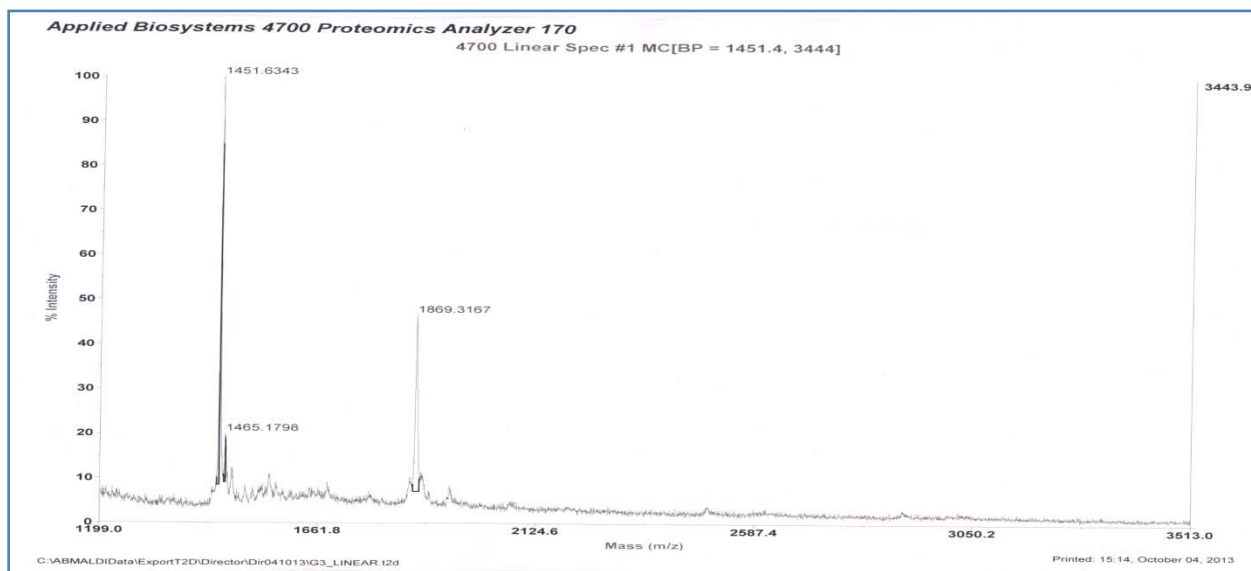
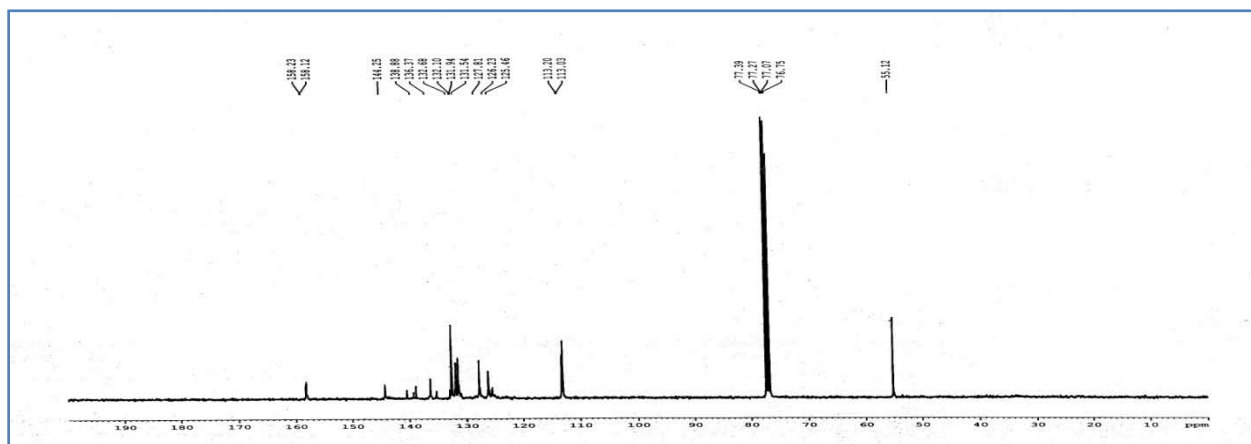
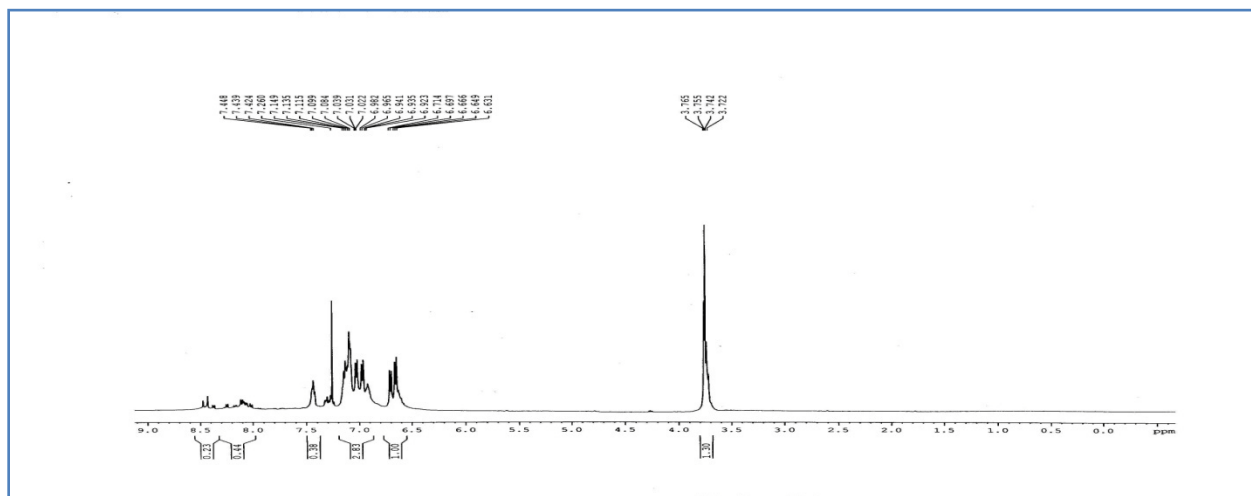
Compound 7:



Compound 8:



Compound 9:



Compound 10:

