Supplementary Information

Synthesis and spectral studies of some bio-active aryl bis-enones

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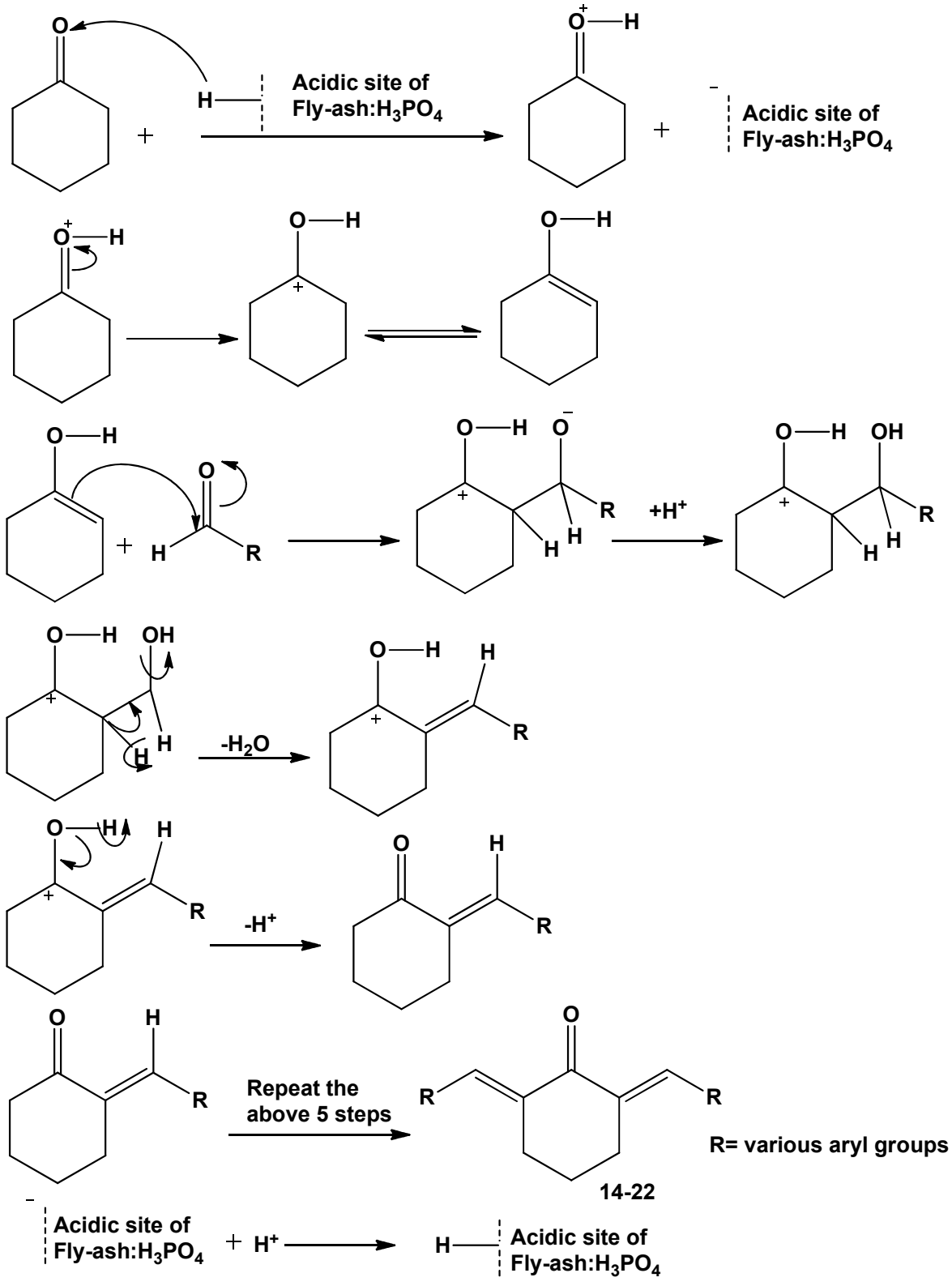
Schemes S1-S6: Mechanistic pathways of synthesis of bis-enones.

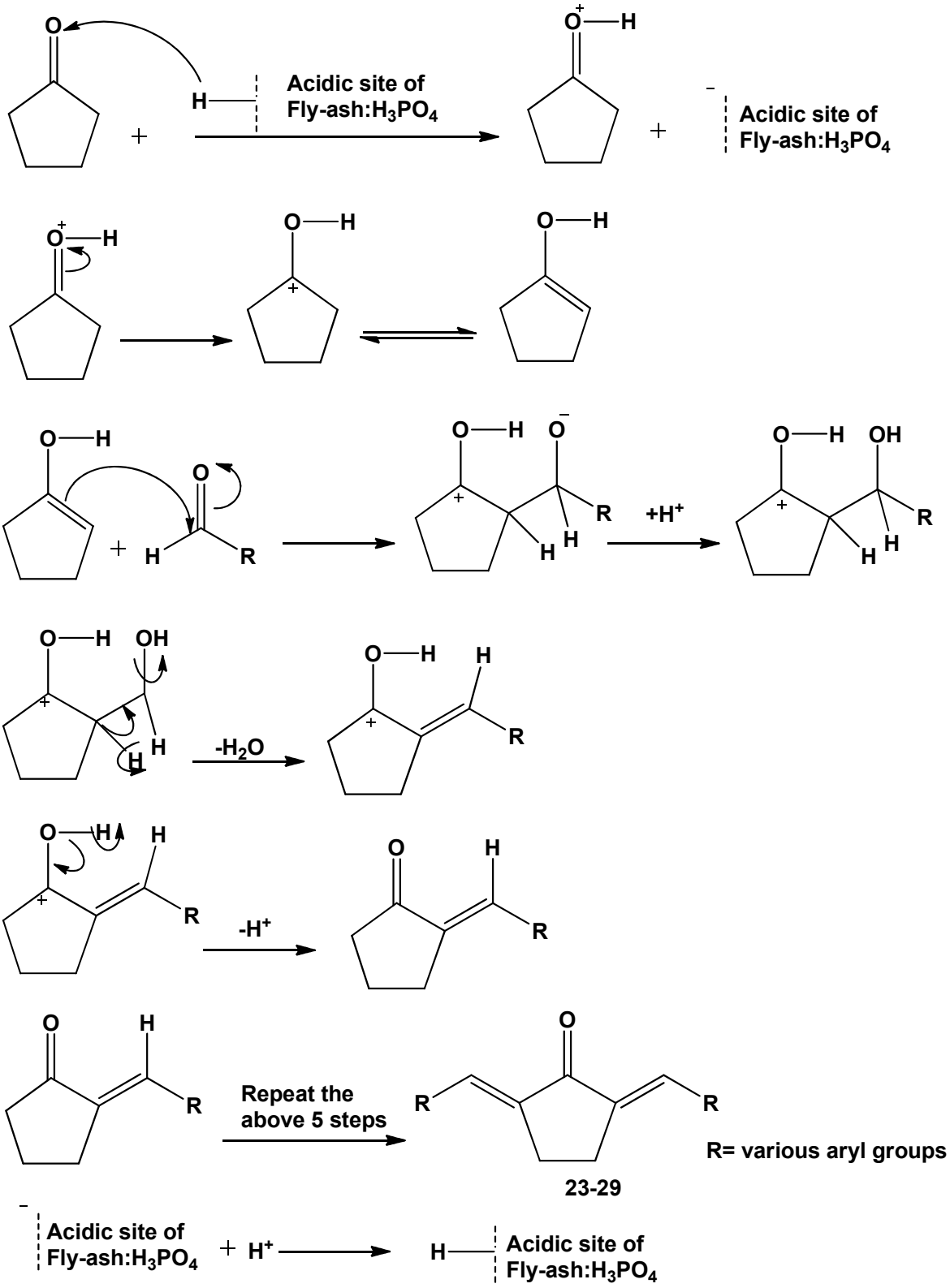
Table S1: Statistical analysis results for correlation study

Table S2: Molecular docking results

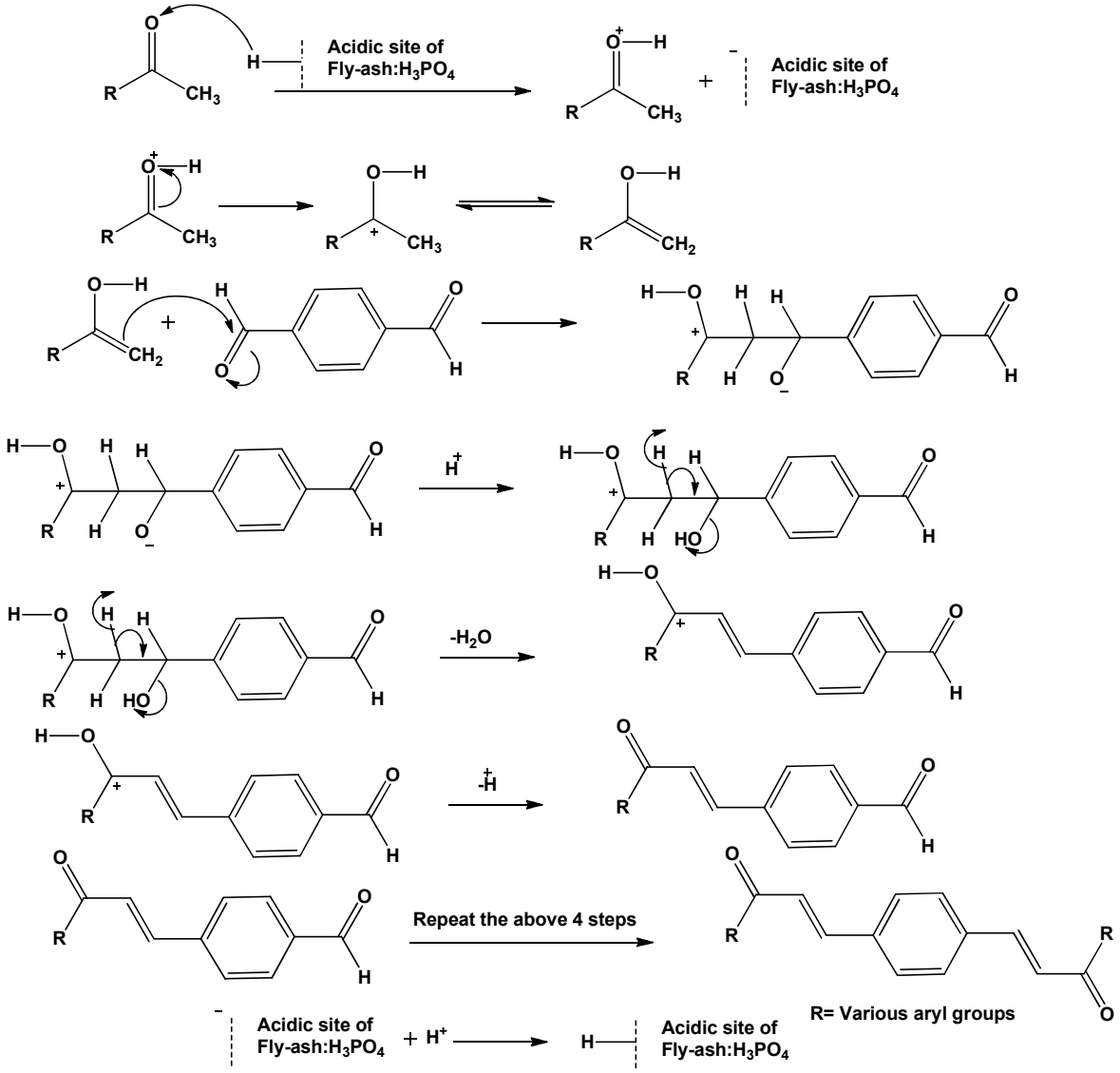
Figure S1a-S7c: NMR spectra of selective bis-chalcones



Scheme S1- Mechanistic path way for the synthesis of bis-enones(14-22)

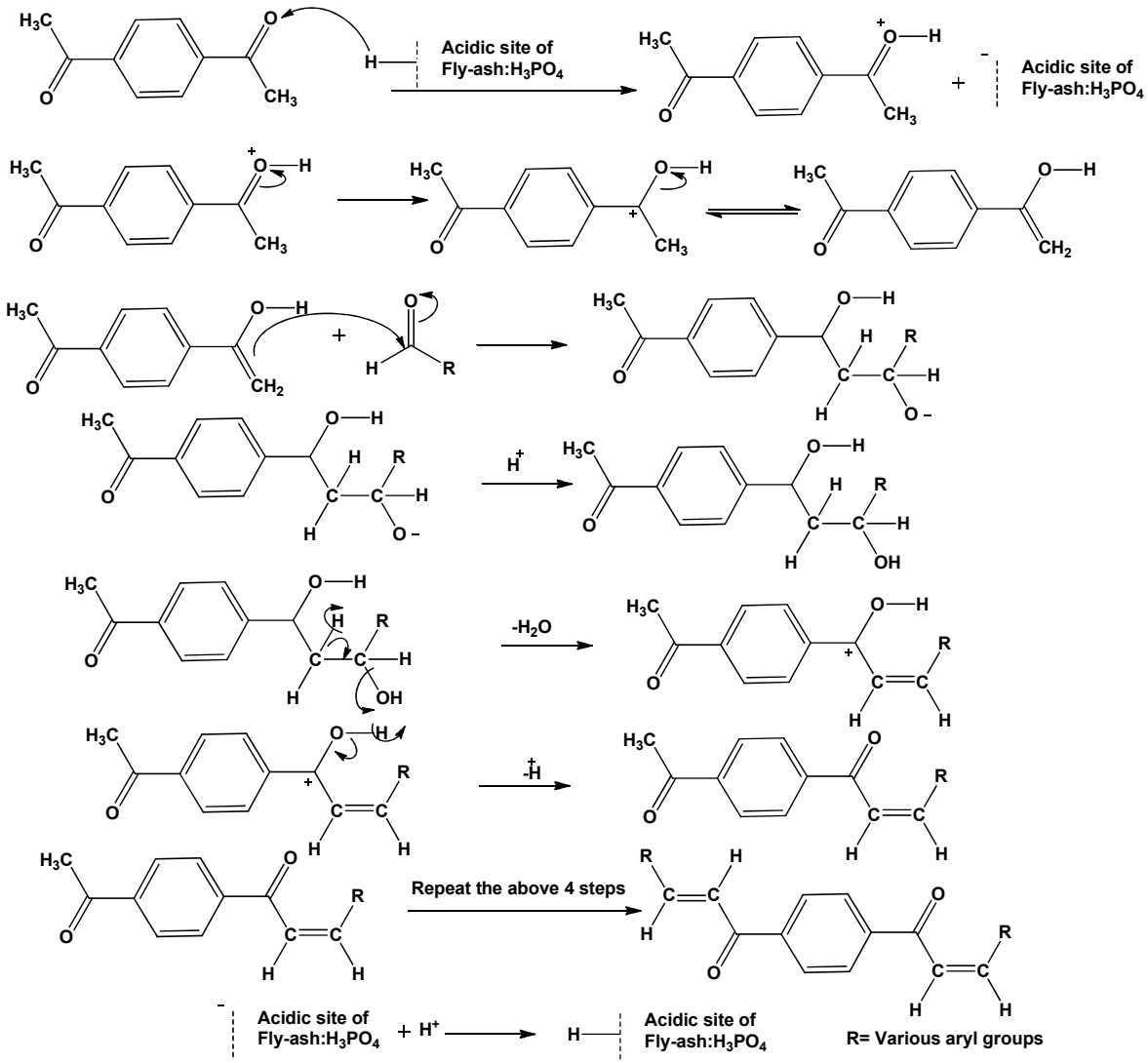


Scheme S2- Mechanistic path way for the synthesis of bis-enones(23-29)



Scheme S3- Mechanistic path way for the synthesis of bis-enones(54-57)

Scheme S4- Mechanistic path way for the synthesis of bis-enones(30-40) by using phenyl-1,3-dialdehyde



Scheme S5- Mechanistic path way for the synthesis of bis-enones (58-59)

Scheme S6- Mechanistic path way for the synthesis of bis-enones (41-53) using 1,3-diacetylbenzene

Table S1- Results of statistical analysis of infrared absorptions (ν, cm^{-1}) and NMR chemical shifts (δ, ppm) of substituted bis-chalcones with Hammett σ, σ+, σ_I, σ_R and F and R parameters.

Freq.	Constt.	r	I	ρ	s	n	Correlated derivatives
			(1*E*, 4*E*)-1,5-Bis(substituted phenyl)penta-1,4-dien-3-ones				
C=O	σ	0.906	1657.71	–44.084	11.43	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.902	1656.29	–19.594	11.32	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.804	1657.22	–5.643	14.47	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.904	1646.80	–35.114	12.98	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.784	1657.15	–4.662	14.48	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	R	0.905	1645.81	–30.90	12.47	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
C=C	σ	0.540	1579.40	4.234	21.19	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.115	1579.44	5.242	21.07	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.025	1578.96	2.213	21.20	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.907	1563.13	–65.646	17.34	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.716	1576.53	–9.447	21.06	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	R	0.906	1562.87	–52.758	16.95	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
H_α	σ	0.769	7.381	0.212	0.61	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.633	7.385	0.179	0.60	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.903	7.393	–0.007	0.61	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.656	7.686	1.176	0.57	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.703	7.388	0.008	0.61	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	R	0.708	7.719	1.033	0.55	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
H_β	σ	0.819	7.277	0.735	0.32	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.767	7.300	0.356	0.31	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.783	7.349	–0.127	0.35	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.856	7.433	0.489	0.34	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.656	7.382	–0.213	0.35	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3

	R	0.893	7.403	0.282	0.50	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
C=O	σ	0.546	189.245	2.727	3.74	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.609	189.260	3.324	3.45	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.481	190.226	–28.370	3.72	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.340	187.637	–6.915	3.55	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.417	189.931	–1.704	3.75	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	R	0.684	187.467	–6.018	3.49	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
C_α	σ	0.901	126.624	0.011	1.99	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.900	126.646	–0.633	1.97	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.055	126.761	–0.457	1.99	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.900	126.544	7.634	1.39	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.241	127.225	–1.834	1.93	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	R	0.907	128.479	5.845	1.40	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
C_β	σ	0.357	141.865	–2.43	1.29	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ^+	0.238	141.774	–0.706	1.34	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_I	0.905	142.635	–2.957	1.18	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	σ_R	0.904	141.759	0.033	1.38	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	F	0.903	142.332	–1.775	1.30	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3
	R	0.901	141.464	–0.899	1.36	8	H, 4–Br, 2–Cl, 4–Cl, 4–F, 3–OCH_3, 4–OCH_3, 4–CH_3

(2*E*, 6*E*)-2,6-Bis(substituted benzylidene)cyclohexanones

C=O	σ	0.901	1671.07	47.624	35.96	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 2–NO_2,
	σ^+	0.904	1676.22	35.555	34.03	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_I	0.901	1655.54	56.006	37.46	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_R	0.903	1686.69	57.059	37.94	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	F	0.901	1660.80	37.981	38.77	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH,

							4–OCH_3, 4– CH_3, 4–NO_2,
	R	0.903	1686.39	41.006	38.16	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
C=C	σ	0.165	1596.15	13.723	30.33	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ^+	0.257	1597.76	13.31	29.71	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_I	0.257	1586.52	11.154	2.715	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_R	0.904	1598.44	5.639	30.72	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	F	0.901	1588.32	22.834	30.14	9	H, 4–Br, 2–Cl, 4-Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	R	0.903	1598.32	3.887	30.73	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 2–NO_2,
H_β	σ	0.905	7.439	0.301	0.28	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ^+	0.903	7.468	0.126	0.29	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_I	0.906	7.473	0.033	0.30	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_R	0.904	7.592	0.626	0.26	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	F	0.905	7.487	–0.066	0.302	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	R	0.905	7.610	0.520	0.259	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
C=O	σ	0.913	189.35	–0.272	0.749	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ^+	0.903	189.33	–0.047	0.755	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_I	0.901	189.73	–1.167	0.695	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_R	0.904	189.36	0.157	0.755	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	F	0.902	189.62	–0.784	0.726	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	R	0.930	189.42	0.334	0.749	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
C_α	σ	0.903	130.103	–2.762	2.605	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ^+	0.904	129.803	–2.115	2.500	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_I	0.901	129.508	1.108	2.785	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_R	0.905	128.495	–6.669	2.357	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	F	0.902	128.914	2.649	2.709	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	R	0.906	128.127	–6.217	2.091	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH,

							4–OCH_3, 4– CH_3, 4–NO_2,
C_β	σ	0.900	137.168	0.697	1.468	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ^+	0.905	137.227	0.012	1.490	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_I	0.903	136.524	2.033	1.397	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	σ_R	0.764	137.133	–0.423	1.487	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	F	0.904	136.294	2.523	1.329	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4– CH_3, 4–NO_2,
	R	0.793	136.949	–0.961	1.462	9	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OH, 4–OCH_3, 4–CH_3, 4–NO_2,

(2*E*,6*E*)-2,6-Bis(substituted benzylidene)cyclopentanones

C=O	σ	0.902	1692.78	5.978	5.278	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ^+	0.906	1693.02	0.702	5.430	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_I	0.908	1687.65	17.272	2.984	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_R	0.907	1688.37	–20.384	3.878	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	F	0.907	1688.21	14.384	3.545	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	R	0.906	1688.74	–15.070	4.090	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
C=C	σ	0.902	1587.10	–6.649	4.982	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ^+	0.901	1536.81	–1.439	5.150	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_I	0.907	1591.33	–14.44	3.534	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_R	0.900	1590.25	14.975	4.372	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	F	0.604	1590.80	–11.850	3.925	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	R	0.905	1590.01	11.178	4.459	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
H_β	σ	0.930	7.611	–0.195	0.028	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ^+	0.936	7.602	–0.070	0.039	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_I	0.904	7.659	–0.177	0.022	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_R	0.903	7.624	0.088	0.049	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	F	0.947	7.655	–0.152	0.027	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3

	R	0.901	7.616	0.095	0.050	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
C=O	σ	0.905	196.26	–0.982	0.523	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ^+	0.905	196.21	–0.470	0.530	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_I	0.907	196.57	–1.118	0.712	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_R	0.848	196.40	0.770	0.348	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	F	0.884	196.48	–0.789	0.584	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	R	0.795	196.32	0.340	0.195	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
C_α	σ	0.806	126.03	–2.877	2.999	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ^+	0.703	1268.85	–2.657	2.804	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_I	0.821	129.00	–0.254	3.064	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_R	0.804	127.99	–4.993	2.919	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	F	0.751	128.39	1.6144	3.030	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	R	0.728	127.87	–3.71	2.935	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
C_β	σ	0.904	137.09	4.727	2.214	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ^+	0.916	137.36	3.350	1.889	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_I	0.162	137.73	–1.512	2.414	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	σ_R	0.936	138.86	7.013	2.065	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	F	0.189	137.80	–1.618	2.402	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3
	R	0.956	138.97	6.025	1.982	7	H, 4–Br, 2–Cl, 4–Cl, 4–F, 4–OCH_3, 4–CH_3

r = correlation coefficient; I = intercept; q = slope; s= standard deviation; n= number of derivatives

Table S2– The molecular docking protein binding interaction results of substituted bis-chalcone

Entry	R	R′	PDB ID	Binding Energy ΔG (Kcalmol^{-1})	Grid X–Y–Z Coordinate
		(1*E*, 4*E*)-1,5-Bis(substituted phenyl)penta-1,4-dien-3-ones			
1	Acetone	Ph	3ERT	– 5.32	60,80,60
2	Acetone	4-BrPh	3ERT	– 5.98	60,80,60
3	Acetone	2-ClPh	3ERT	– 5.56	60,80,60
4	Acetone	4-ClPh	3ERT	– 6.77	60,80,60
5	Acetone	4-FPh	3ERT	– 7.88	60,80,60
6	Acetone	4-OCH_3Ph	3ERT	– 7.67	60,80,60
7	Acetone	4-MePh	3ERT	– 6.88	60,80,60
8	Acetone	9-Anthryl	3ERT	– 6.21	60,80,60
9	Acetone	4-BiPh	3ERT	– 6.9	60,80,60
10	Acetone	2,3-Cl_2Ph	3ERT	–5.94	60,80,60
11	Acetone	2-Ferrocene	3ERT	–7.99	60,80,60
12	Acetone	3-OCH_3Ph	3ERT	– 6.88	60,80,60
13	Acetone	1-Pyreneyl	3ERT	– 9.18	60,80,60
		(2*E*, 6*E*)-2,6-Bis(substituted benzylidene)cyclohexanones			
14	Cyclohexanone	Ph	3ERT	–6.33	60,80,60
15	Cyclohexanone	4-BrPh	3ERT	–5.77	60,80,60
16	Cyclohexanone	2-ClPh	3ERT	–6.87	60,80,60
17	Cyclohexanone	4-ClPh	3ERT	–5.33	60,80,60
18	Cyclohexanone	4-FPh	3ERT	–5.43	60,80,60
19	Cyclohexanone	4–OHPh	3ERT	–6.55	60,80,60
20	Cyclohexanone	4-OCH_3Ph	3ERT	–5.45	60,80,60

21	Cyclohexanone	4–CH_3Ph	3ERT	–5.66	60,80,60
22	Cyclohexanone	4–NO_2Ph	3ERT	–5.88	60,80,60
	(2*E*,6*E*)-2,6-Bis(substituted benzylidene)cyclopentanones				
23	Cyclopentanone	Ph	3ERT	–5.21	60,80,60
24	Cyclopentanone	4–BrPh	3ERT	–5.0	60,80,60
25	Cyclopentanone	2–ClPh	3ERT	–5.78	60,80,60
26	Cyclopentanone	4–ClPh	3ERT	–6.0	60,80,60
27	Cyclopentanone	4–FPh	3ERT	–5.31	60,80,60
28	Cyclopentanone	4–OCH_3Ph	3ERT	–6.31	60,80,60
29	Cyclopentanone	4–CH_3Ph	3ERT	–5.66	60,80,60
	(2*E*, 2'*E*)-3,3'-(1,3-Phenylene)bis(1-(substituted phenyl)prop-2-en-1-ones)				
30	Isophthaladehyde	Ph	1M17	–5.77	60,80,60
31	Isophthaladehyde	4–BrPh	1M17	–5.33	60,80,60
32	Isophthaladehyde	4–ClPh	1M17	–6.53	60,80,60
33	Isophthaladehyde	4–FPh	1M17	–5.33	60,80,60
34	Isophthaladehyde	2-Furayl	1M17	–5.23	60,80,60
35	Isophthaladehyde	3,4–$(OCH_3)_2$Ph	1M17	–5.44	60,80,60
36	Isophthaladehyde	4–OCH_3Ph	1M17	–5.56	60,80,60
37	Isophthaladehyde	4–CH_3Ph	1M17	–5.88	60,80,60
38	Isophthaladehyde	2-Thienyl	1M17	–5.11	60,80,60
39	Isophthaladehyde	2,4–$(OCH_3)_2$Ph	1SA0	–5.23	60,80,60
40	Isophthaladehyde	2,4–$(OH)_2$Ph	1SA0	–5.11	60,80,60
	(2*E*, 2'*E*)-1,1'-(1,3-Phenylene)bis(3-(substitutedphenyl)prop-2-en-1-one)				
41	1,1'-(1,3-phenylene)diethanone	Ph	1M17	–5.88	60,80,60
42	1,1'-(1,3-phenylene)diethanone	4–BrPh	1M17	–5.08	60,80,60

43	1,1'-(1,3-phenylene)diethanone	4–ClPh	1M17	–5.55	60,80,60
44	1,1'-(1,3-phenylene)diethanone	4–FPh	1M17	–5.34	60,80,60
45	1,1'-(1,3-phenylene)diethanone	2-Furyl	1M17	–5.99	60,80,60
46	1,1'-(1,3-phenylene)diethanone	3,4–OCH_3Ph	1M17	–6.88	60,80,60
47	1,1'-(1,3-phenylene)diethanone	4–OCH_3Ph	1M17	–7.85	60,80,60
48	1,1'-(1,3-phenylene)diethanone	4–CH_3Ph	1M17	–6.33	60,80,60
49	1,1'-(1,3-phenylene)diethanone	2-Thienyl	1M17	–5.55	60,80,60
50	1,1'-(1,3-phenylene)diethanone	2,4–$(OCH_3)_2$Ph	1SA0	–5.62	60,80,60
51	1,1'-(1,3-phenylene)diethanone	2,4–$(OH)_2$Ph	5XDL	–6.24	60,80,60
52	1,1'-(1,3-phenylene)diethanone	3,4–$(OH)_2$Ph	5XDL	–4.11	60,80,60
53	1,1'-(1,3-phenylene)diethanone	4-OHPh	5XDL	–4.21	60,80,60
	(2*E*,2'*E*)-3,3'-(1,4-Phenylene)bis(1-(substituted phenyl)prop-2-en-1-ones)				
54	Terephthalaldehyde	2,4–$(OCH_3)_2$Ph	1SA0	–5.62	60,80,60
55	Terephthalaldehyde	3,4–$(OCH_3)_2$Ph	1SA0	–6.48	60,80,60
56	Terephthalaldehyde	2,4-$(OH)_2$Ph	5XDL	–8.01	60,80,60
57	Terephthalaldehyde	3,4-$(OH)_2$Ph	5XDL	–5.22	60,80,60
	(2*E*,2'*E*)-1,1'-(1,4-Phenylene)bis(3-(substituted phenyl)prop-2-en-1-ones)				
58	1,1'-(1,4-phenylene)diethanone	2,4–$(OCH_3)_2$Ph	1SA0	–5.82	60,80,60
59	1,1'-(1,4-phenylene)diethanone	2,4-–$(OH)_2$Ph	5XDL	–5.11	60,80,60

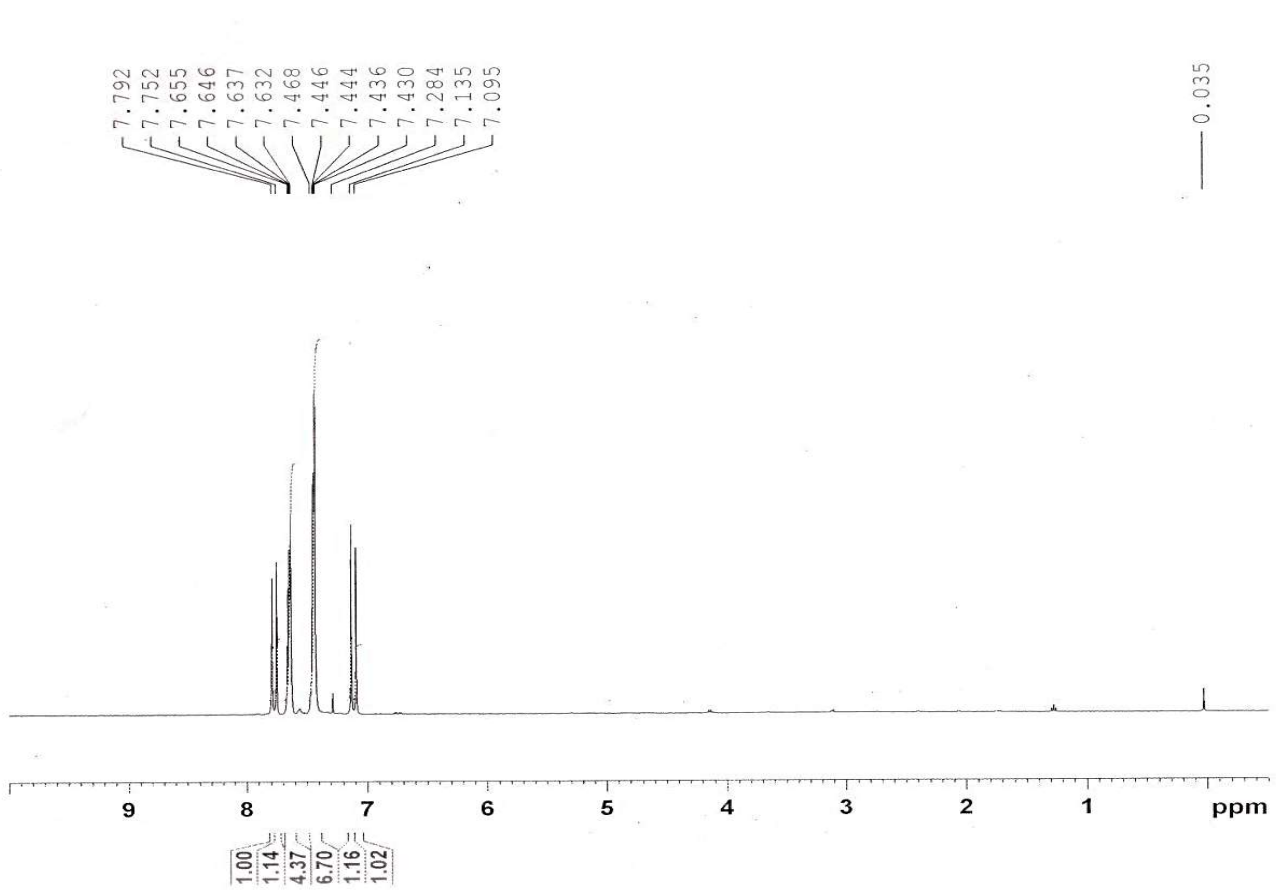



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Figure S1a. ^{1}H NMR spectra of Dibenzalacetone (1)

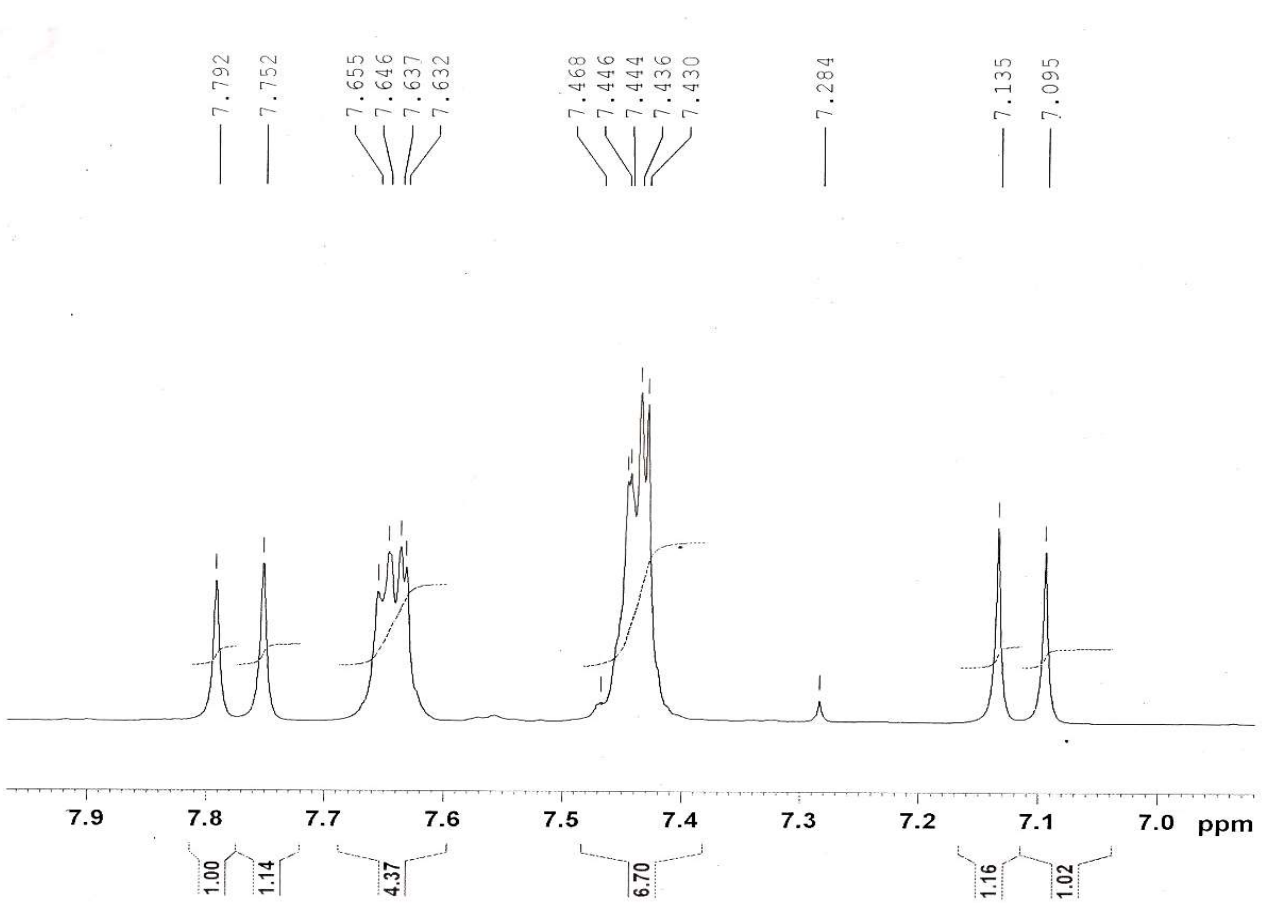


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Figure S1b. ^{1}H NMR spectra of Dibenzalacetone (1) (Scanned)

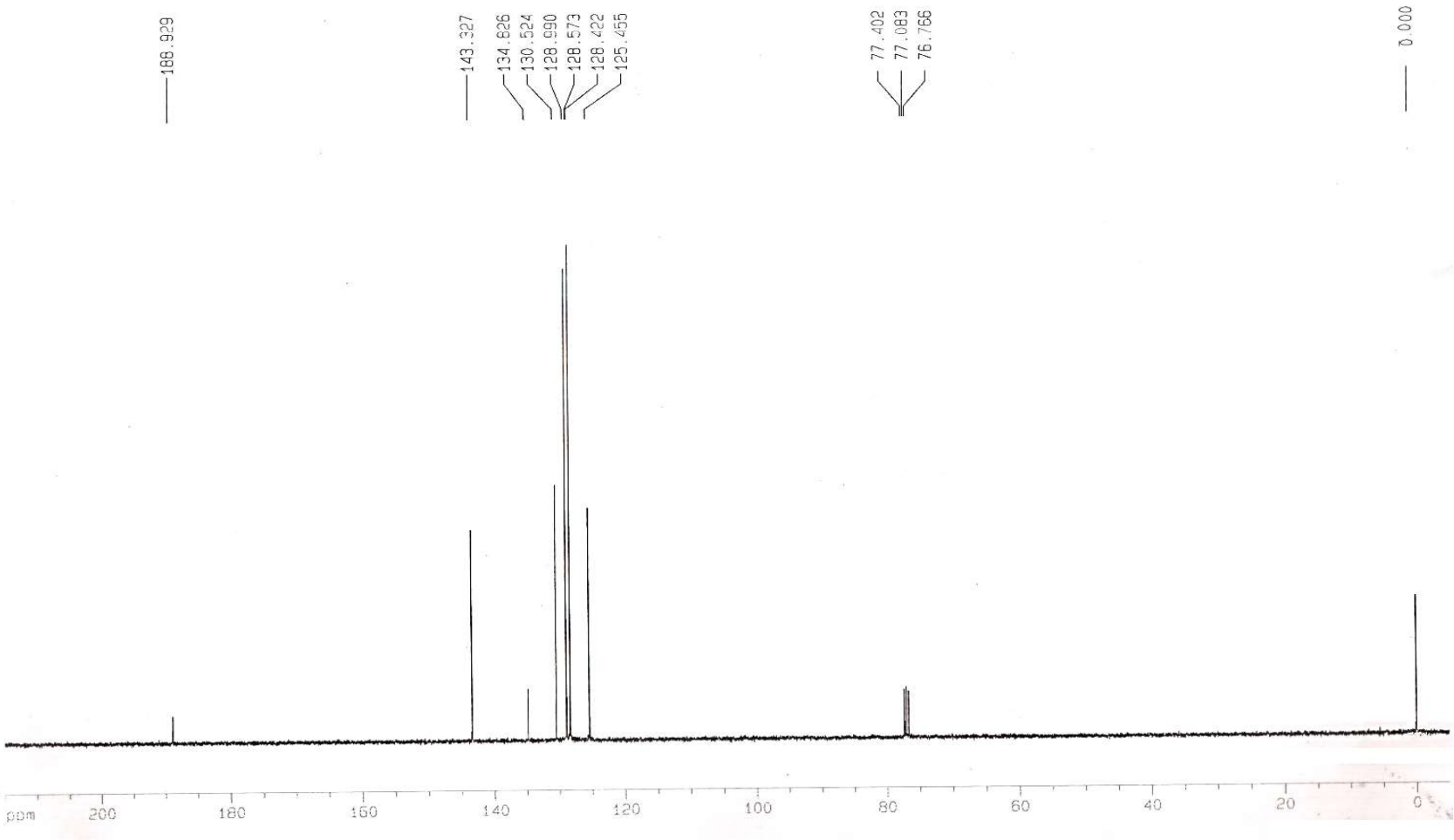

Figure S1c. ^{13}C NMR spectra of Dibenzalacetone (1)

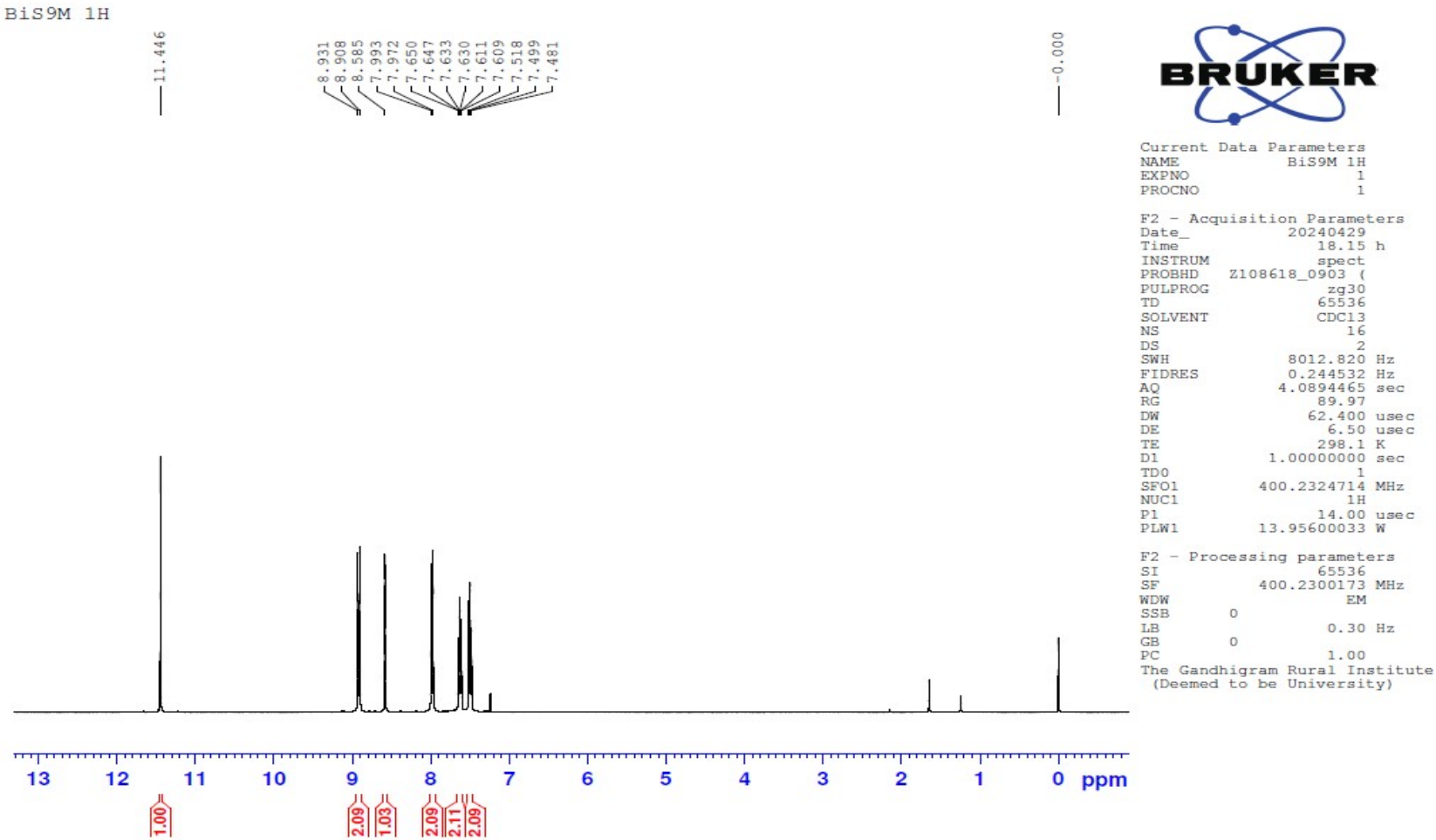

Figure S2a. ^{1}H NMR spectra of *(1Z,4Z)*-1,5-di(anthracen-9-yl) penta-1,4-dien-3-one (8)

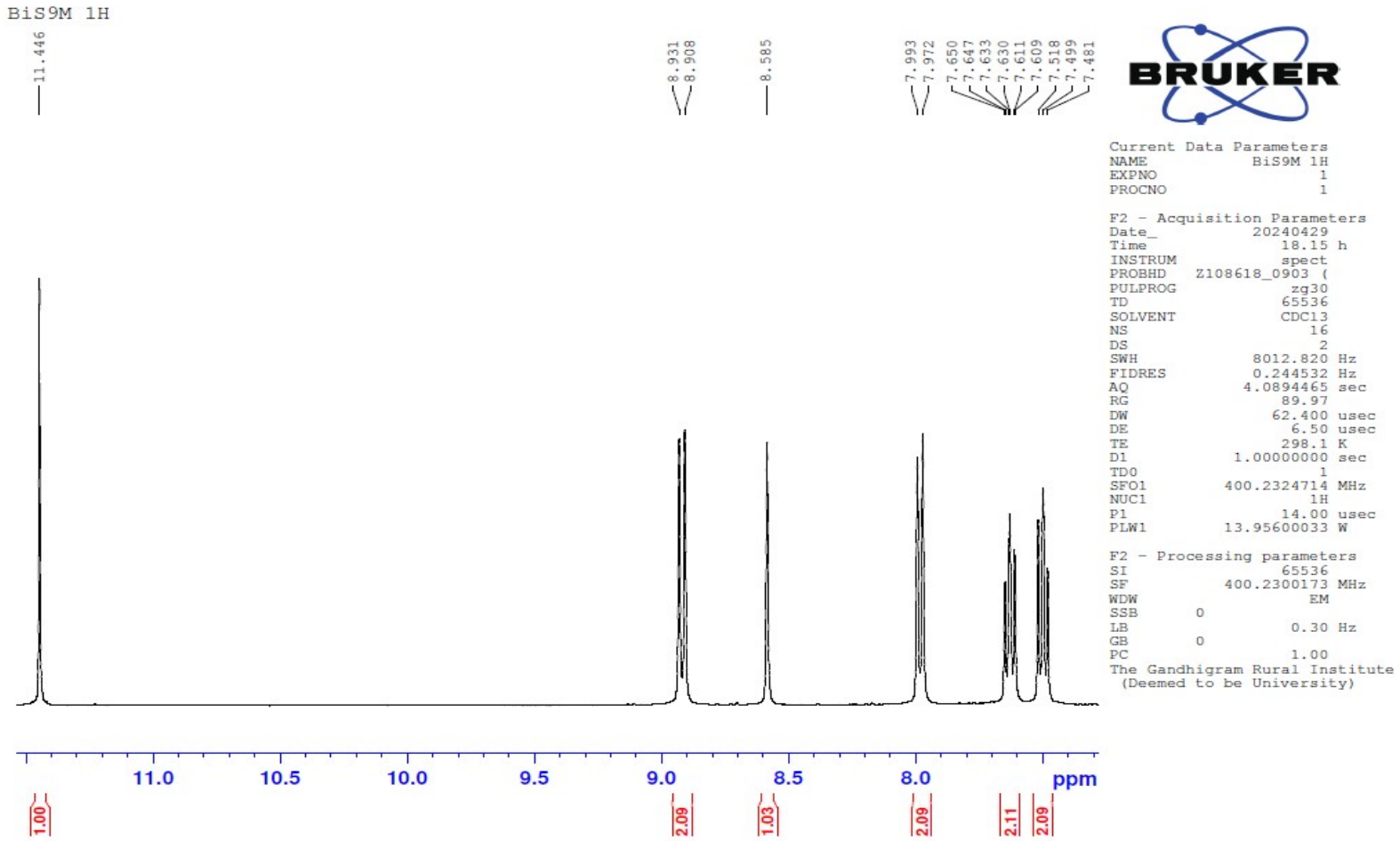

Figure S2b. ^{1}H NMR spectra of (*1Z,4Z)*-1,5-di(anthracen-9-yl) penta-1,4-dien-3-one (8) (Scanned)

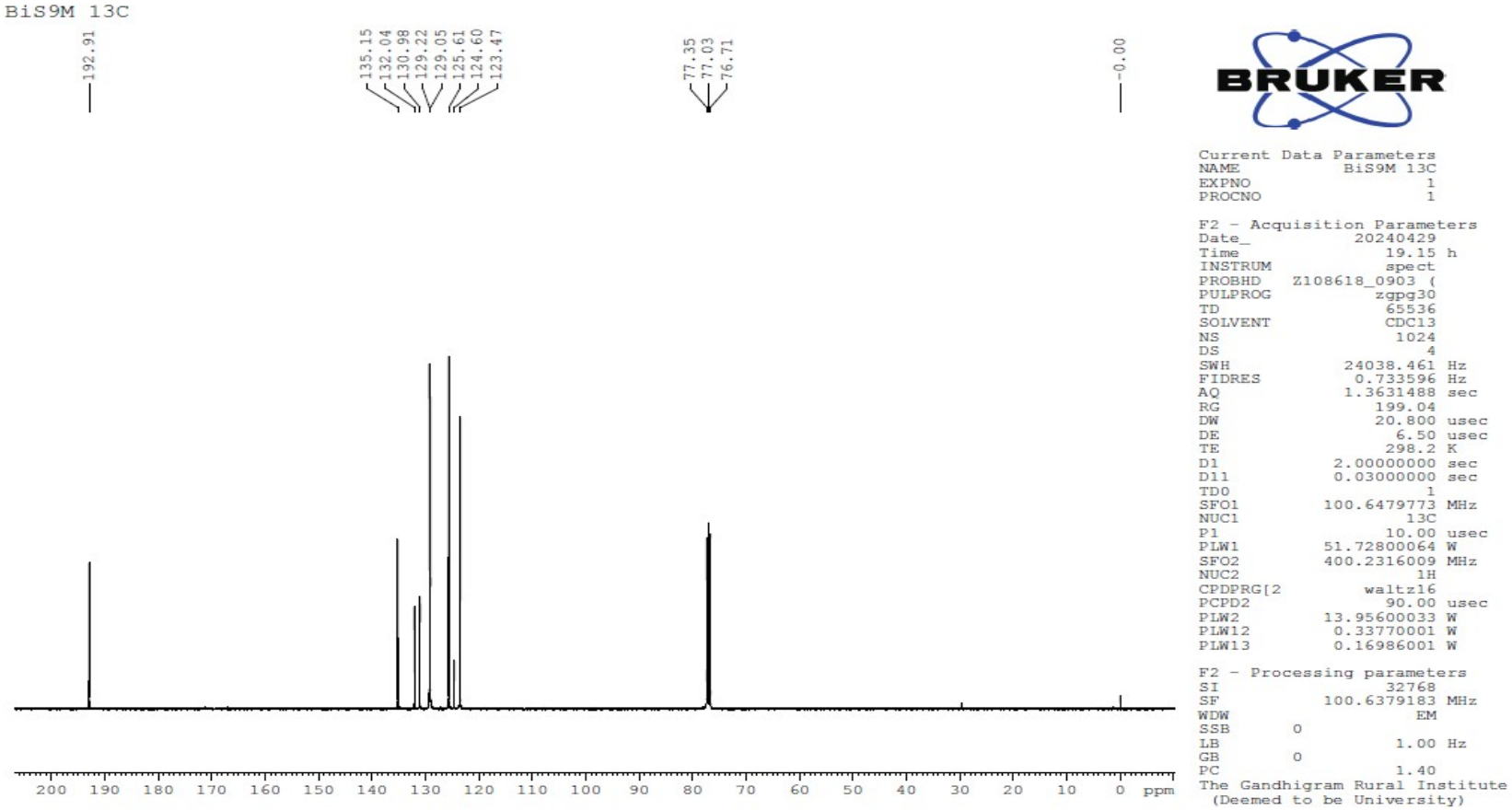

Figure S2c. ^{13}C NMR spectra of (*1Z,4Z)*-1,5-di(anthracen-9-yl) penta-1,4-dien-3-one (8)

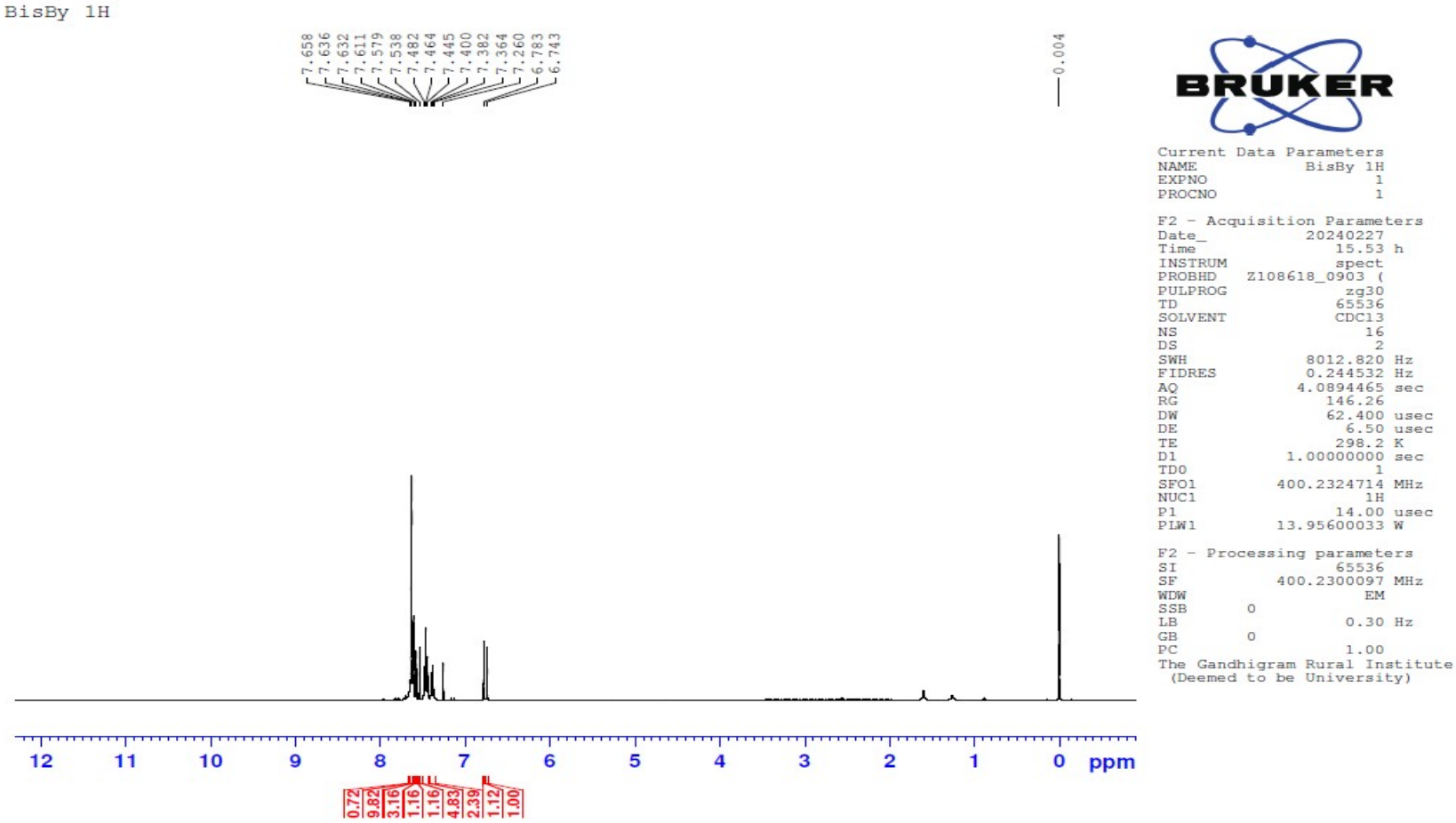

Figure S3a. ^{1}H NMR spectra of (1*E*,4*E*)-1,5-di([1,1'-biphenyl]-4-yl) penta-1,4-dien-3-one (9)

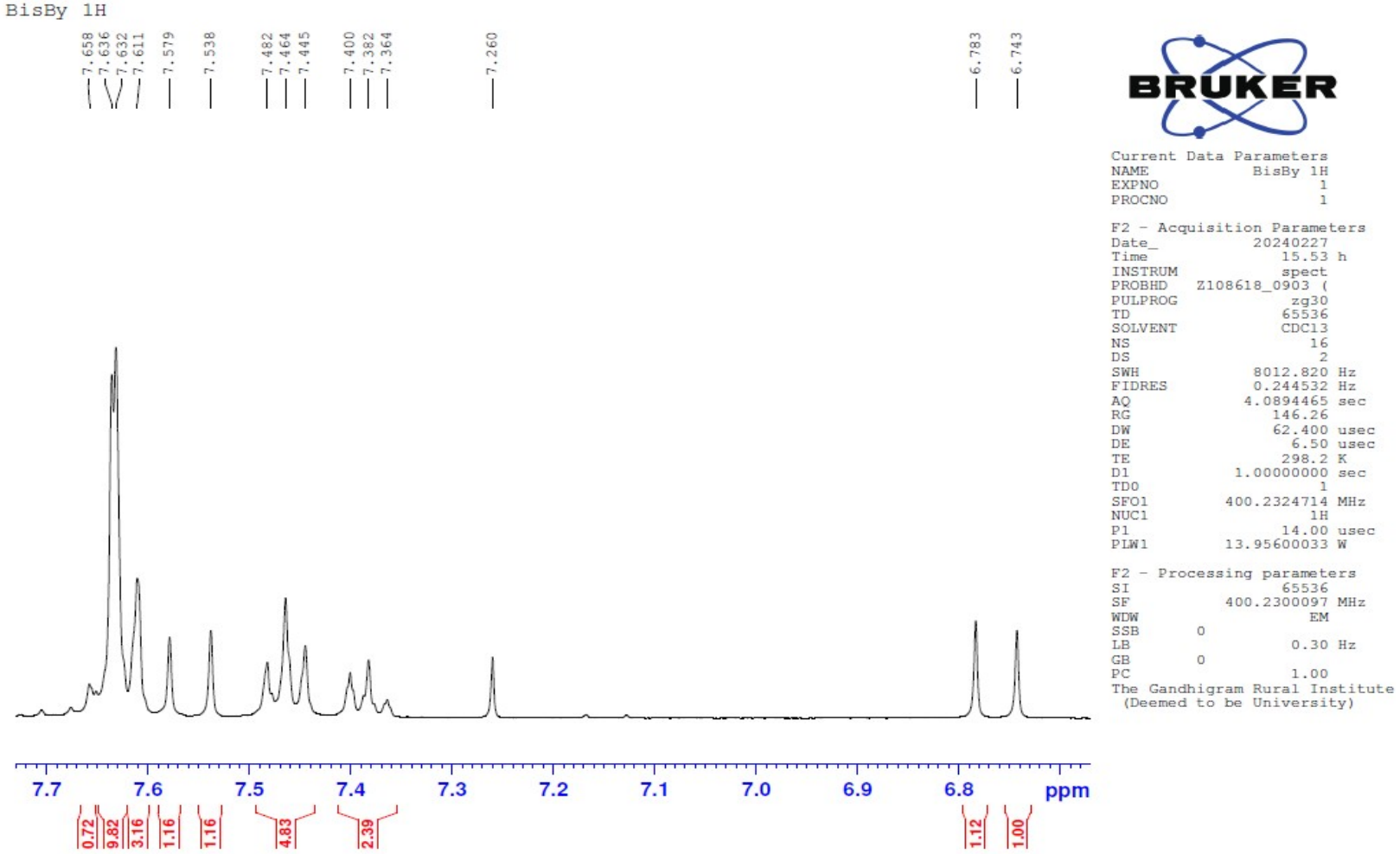

Figure S3b. ^{1}H NMR spectra of (1*E*,4*E*)-1,5-di([1,1'-biphenyl]-4-yl) penta-1,4-dien-3-one (9) (Scanned)

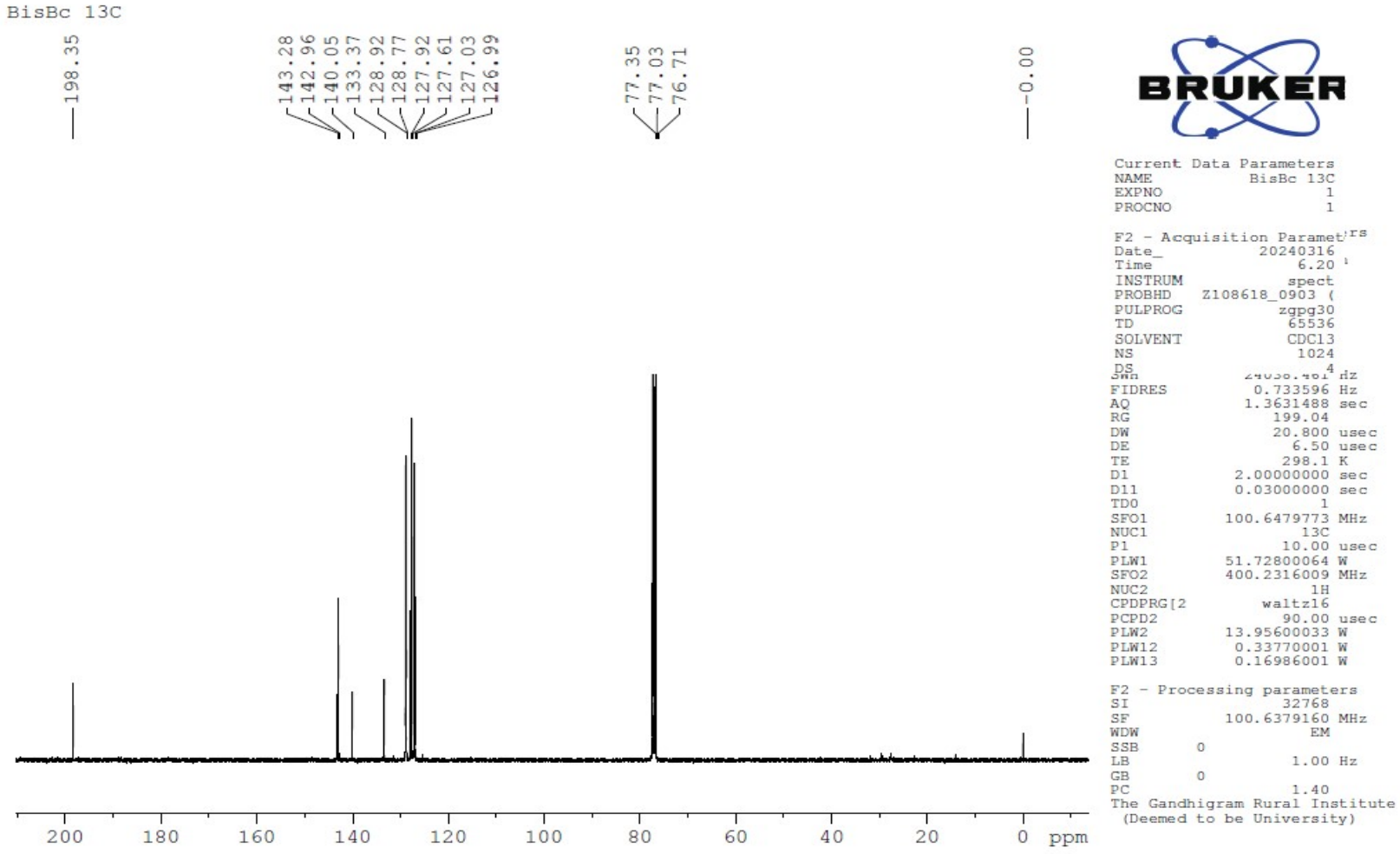

Figure S3c. ^{13}C NMR spectra of (1*E*,4*E*)-1,5-di([1,1'-biphenyl]-4-yl) penta-1,4-dien-3-one (9)

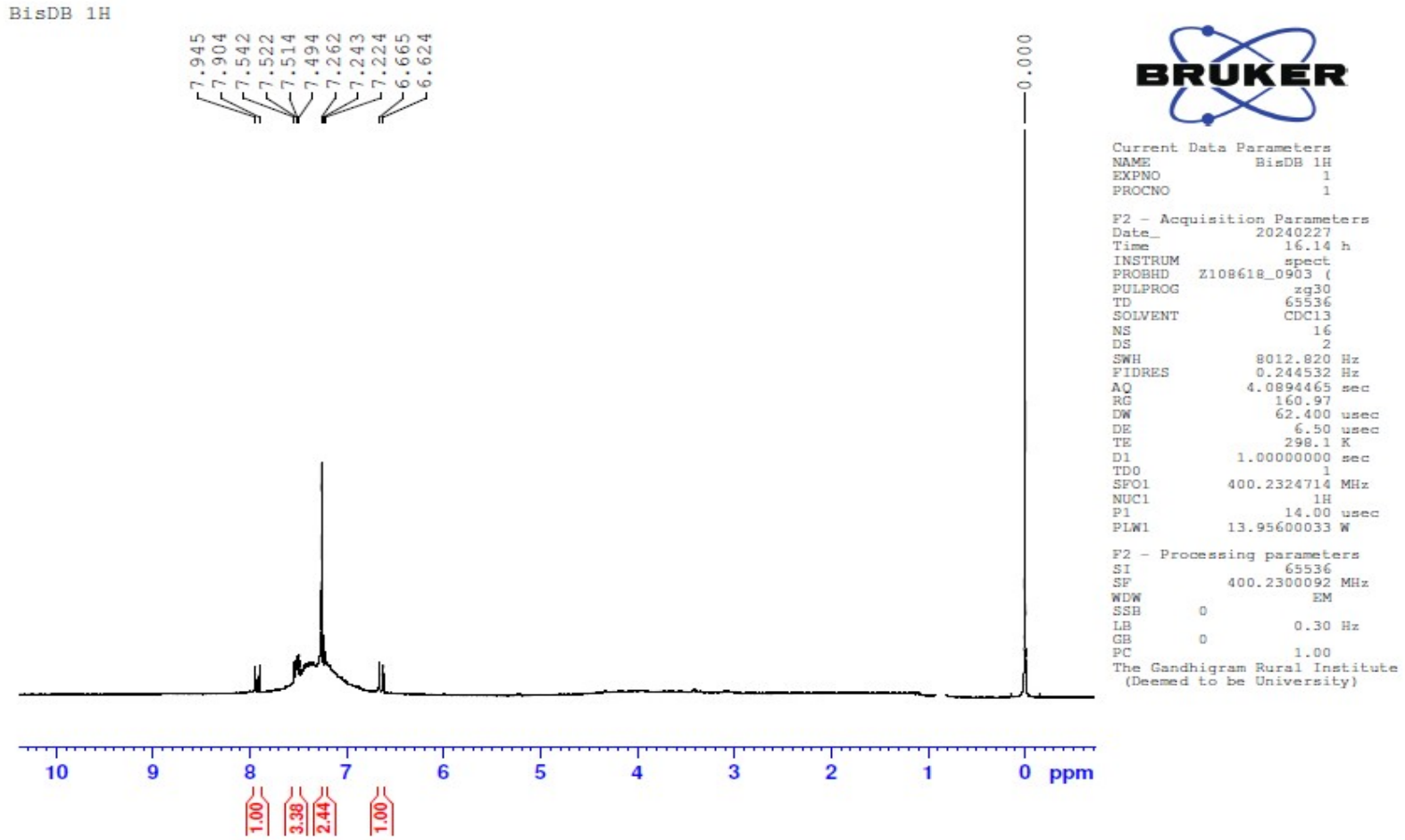

Figure S4a. ^{1}H NMR spectra of (1*E*,4*E*)-1,5-bis(2,3-dichlorophenyl) penta-1,4-dien-3-one (10)

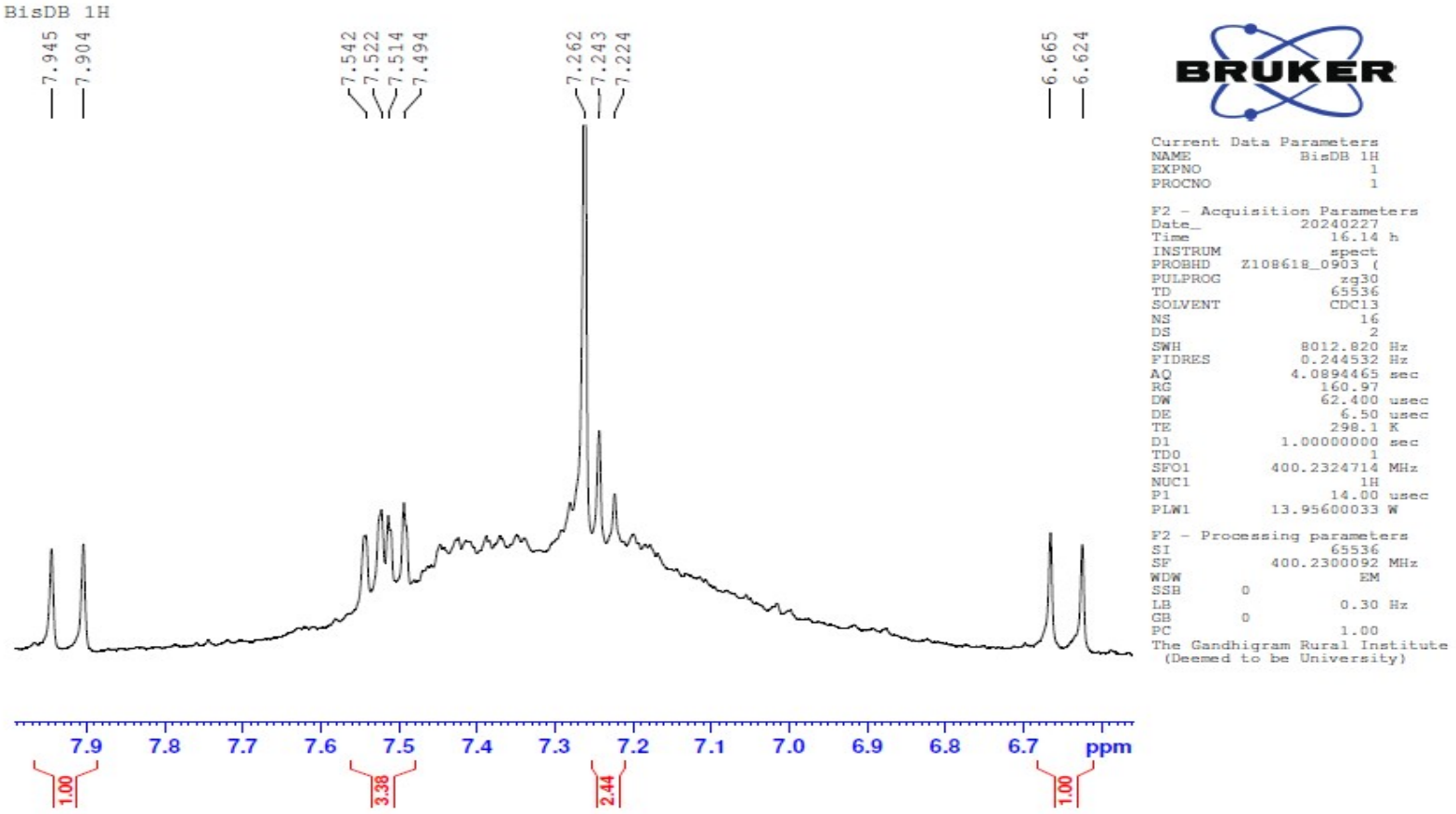

Figure S4b. ^{1}H NMR spectra of (1*E*,4*E*)-1,5-bis(2,3-dichlorophenyl) penta-1,4-dien-3-one (10) (Scanned)

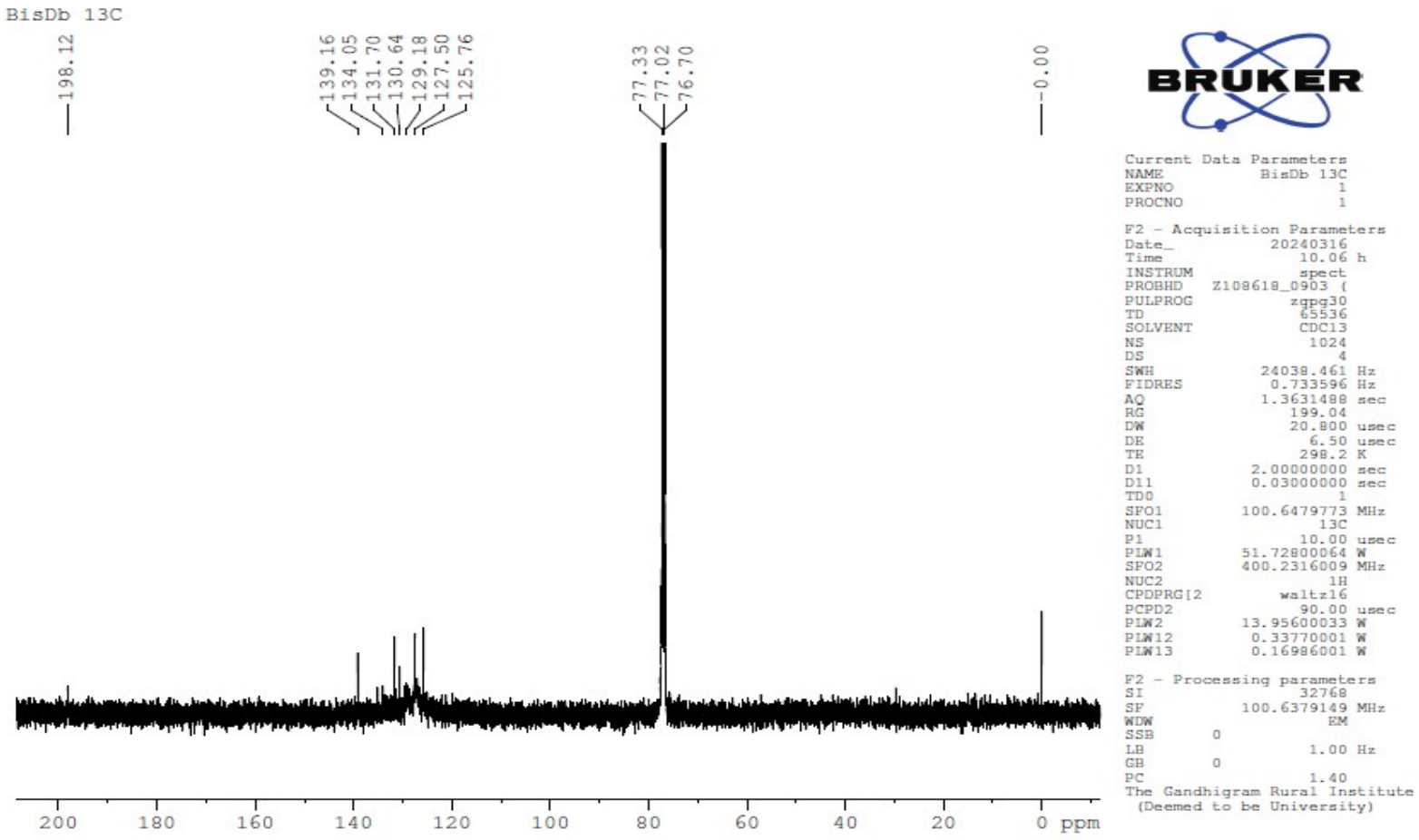

Figure S4c. ^{13}C NMR spectra of (1*E*,4*E*)-1,5-bis(2,3-dichlorophenyl) penta-1,4-dien-3-one (10)

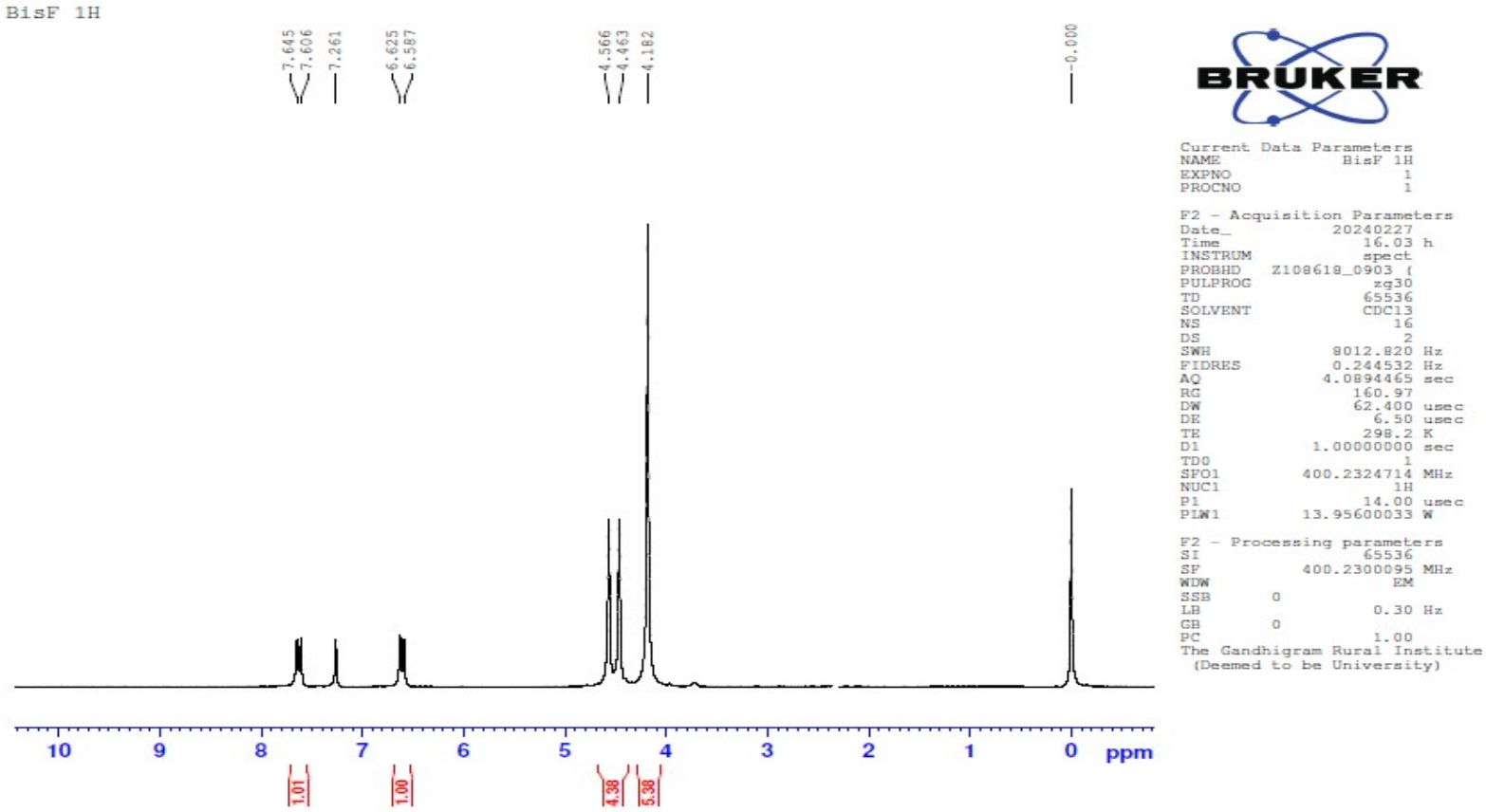

Figure S5a. ^{1}H NMR spectra of (1*E*,4*E*) –1,5–bis(ferrocene)penta –1,4–dien–3–one: (11)

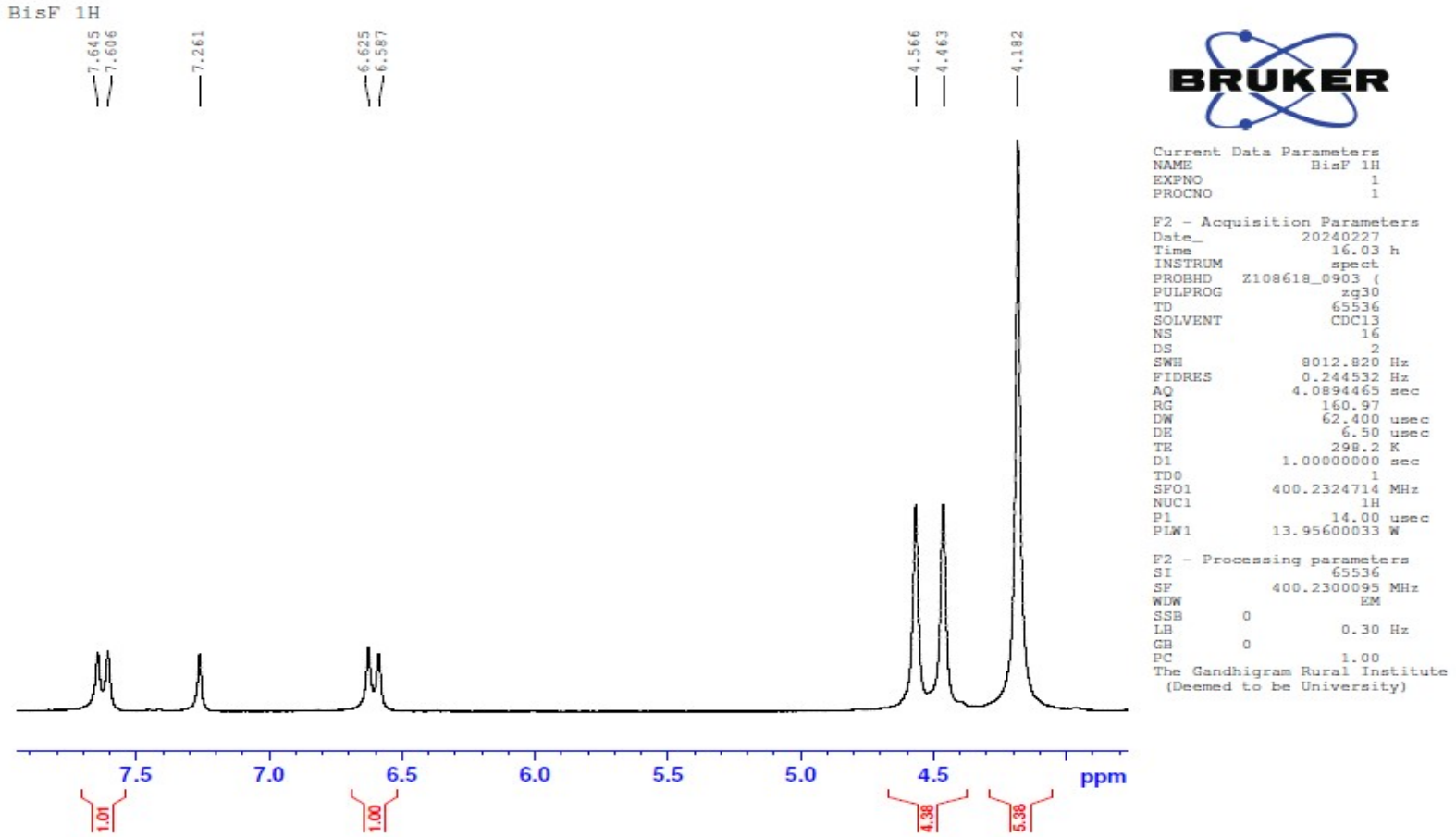

Figure S5b. ^{1}H NMR spectra of (1*E*,4*E*) –1,5–bis(ferrocene)penta –1,4–dien–3–one (11) (Scanned)

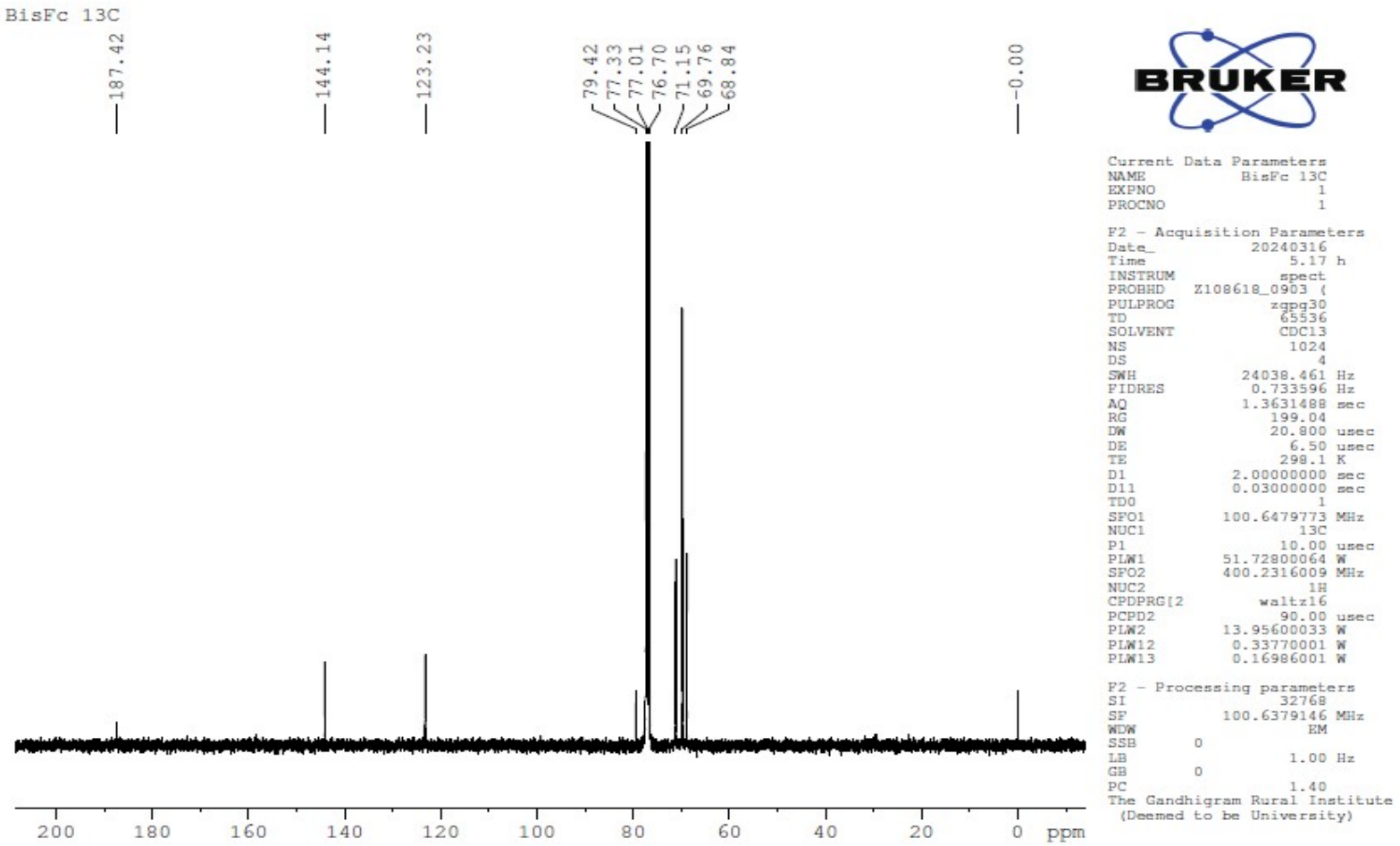

Figure S5c. ^{13}C NMR spectra of (1*E*,4*E*) –1,5–bis(ferrocene)penta –1,4–dien–3–one (11)

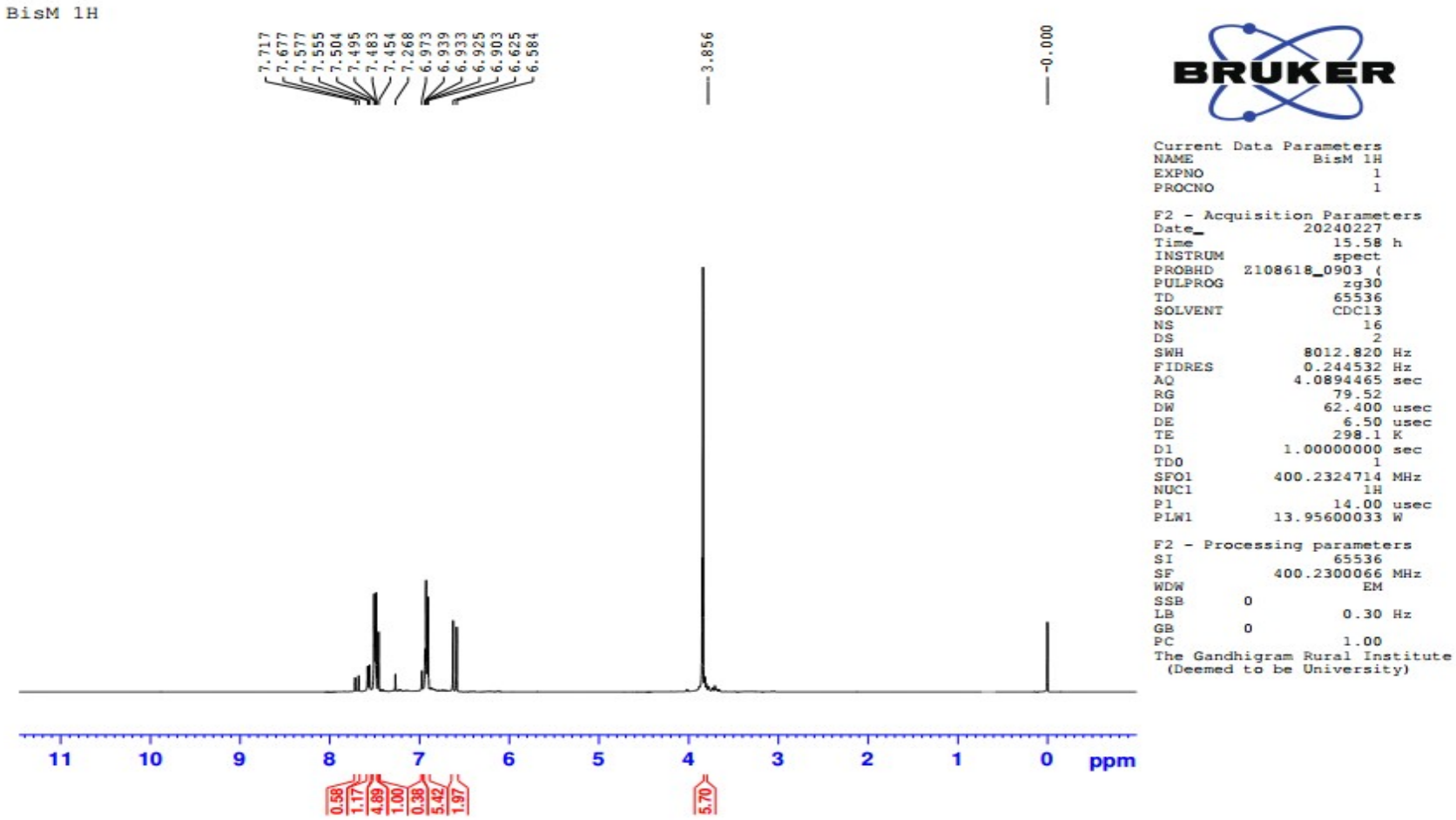

Figure S6a. ^{1}H NMR spectra of (1*E*,4*E*)-1,5-bis(3–methoxyphenyl) penta-1,4-dien-3-one: (12)

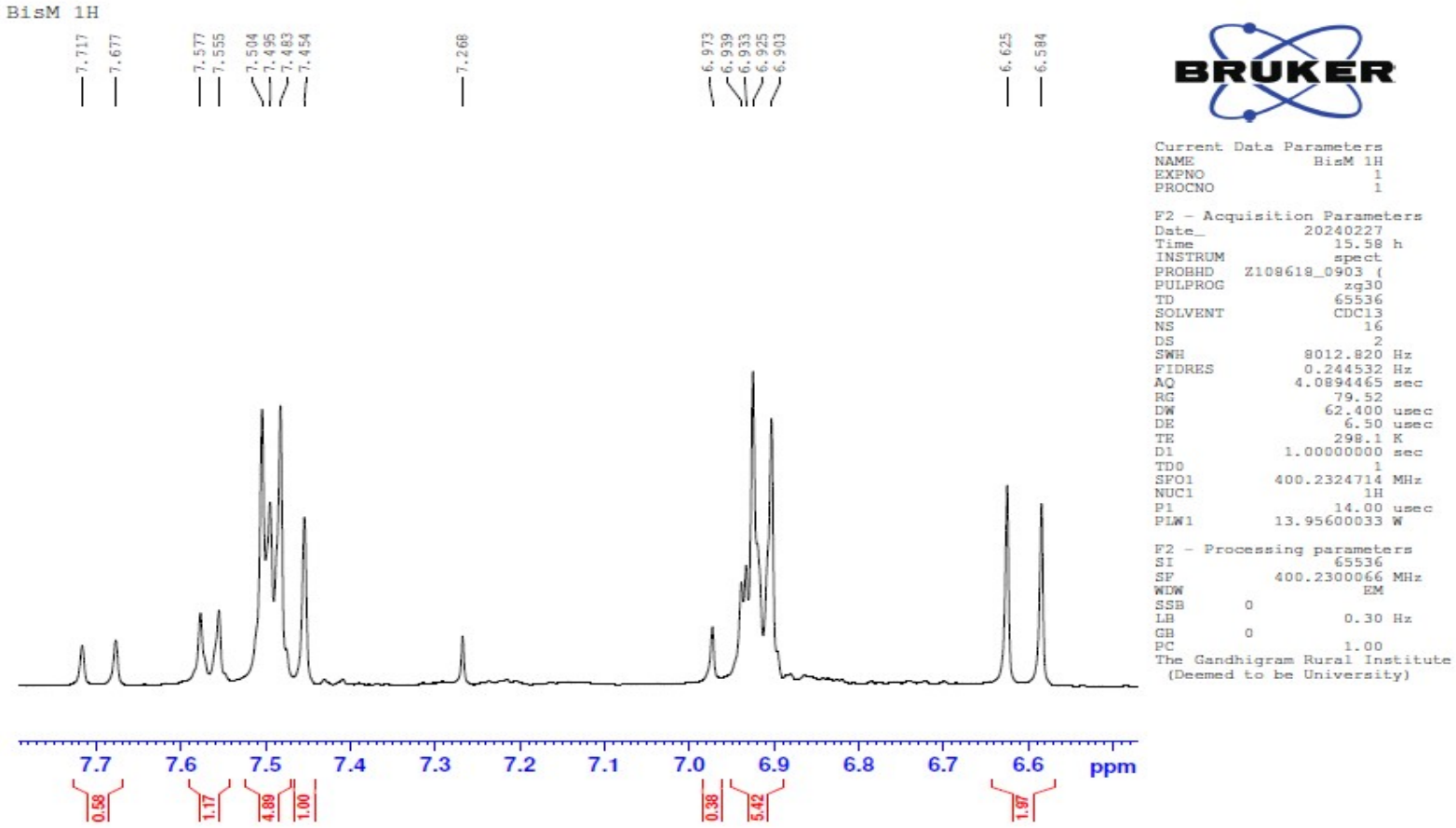

Figure S6b. ^{1}H NMR spectra of (1*E*,4*E*)-1,5-bis(3–methoxyphenyl) penta-1,4-dien-3-one (12) (Scanned)

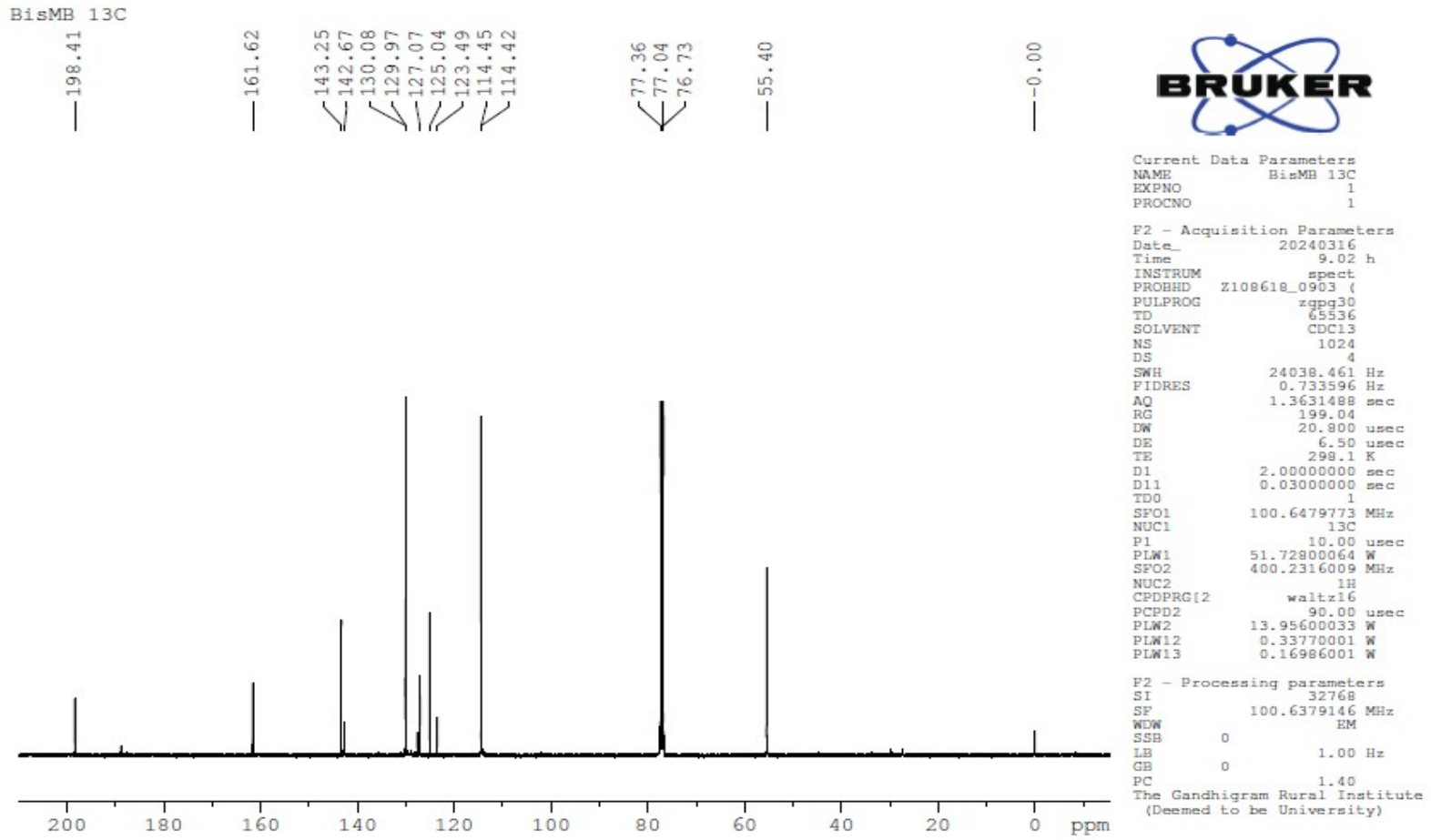

Figure S6c. ^{13}C NMR spectra of (1*E*,4*E*)-1,5-bis(3–methoxyphenyl) penta-1,4-dien-3-one (12)

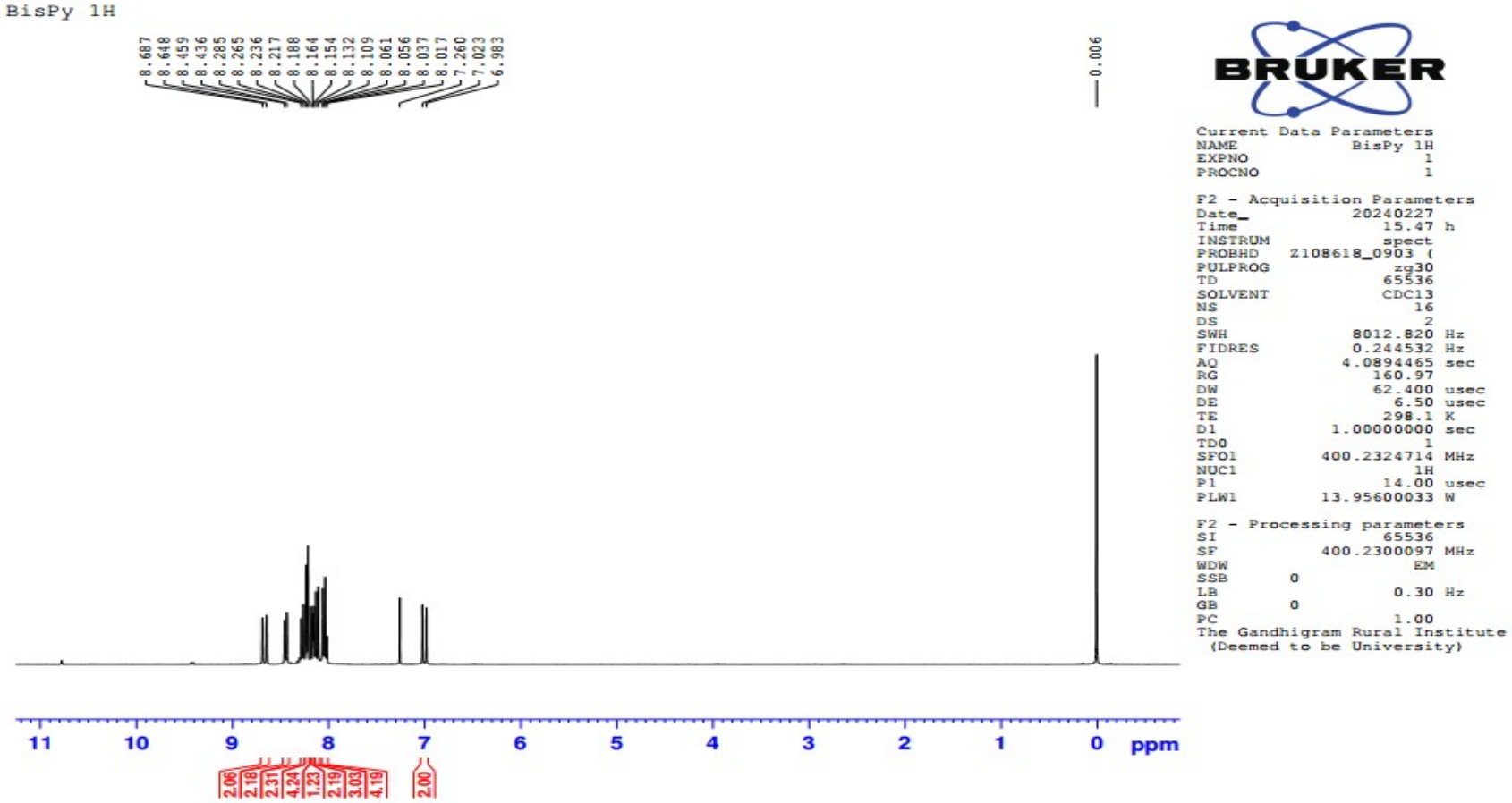

Figure S7a. ^{1}H NMR spectra of (1*E*,4*E*)-1-(4,6-dihydropyren-2-yl)-5-(pyren-4-yl) penta-1,4-dien-3-one: (13)

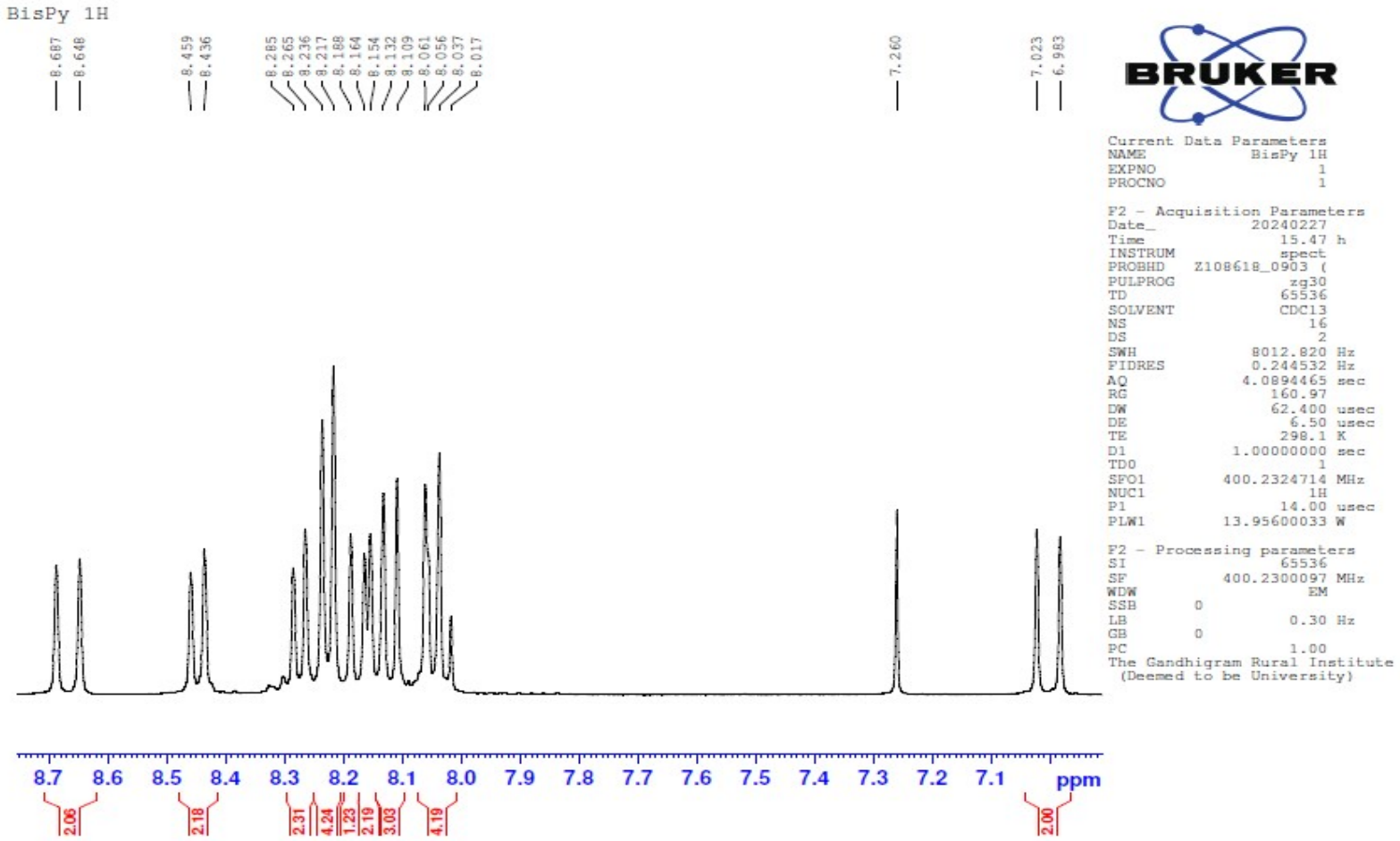

Figure S7b. ^{1}H NMR spectra of (1*E*,4*E*)-1-(4,6-dihydropyren-2-yl)-5-(pyren-4-yl) penta-1,4-dien-3-one (13) (Scanned)

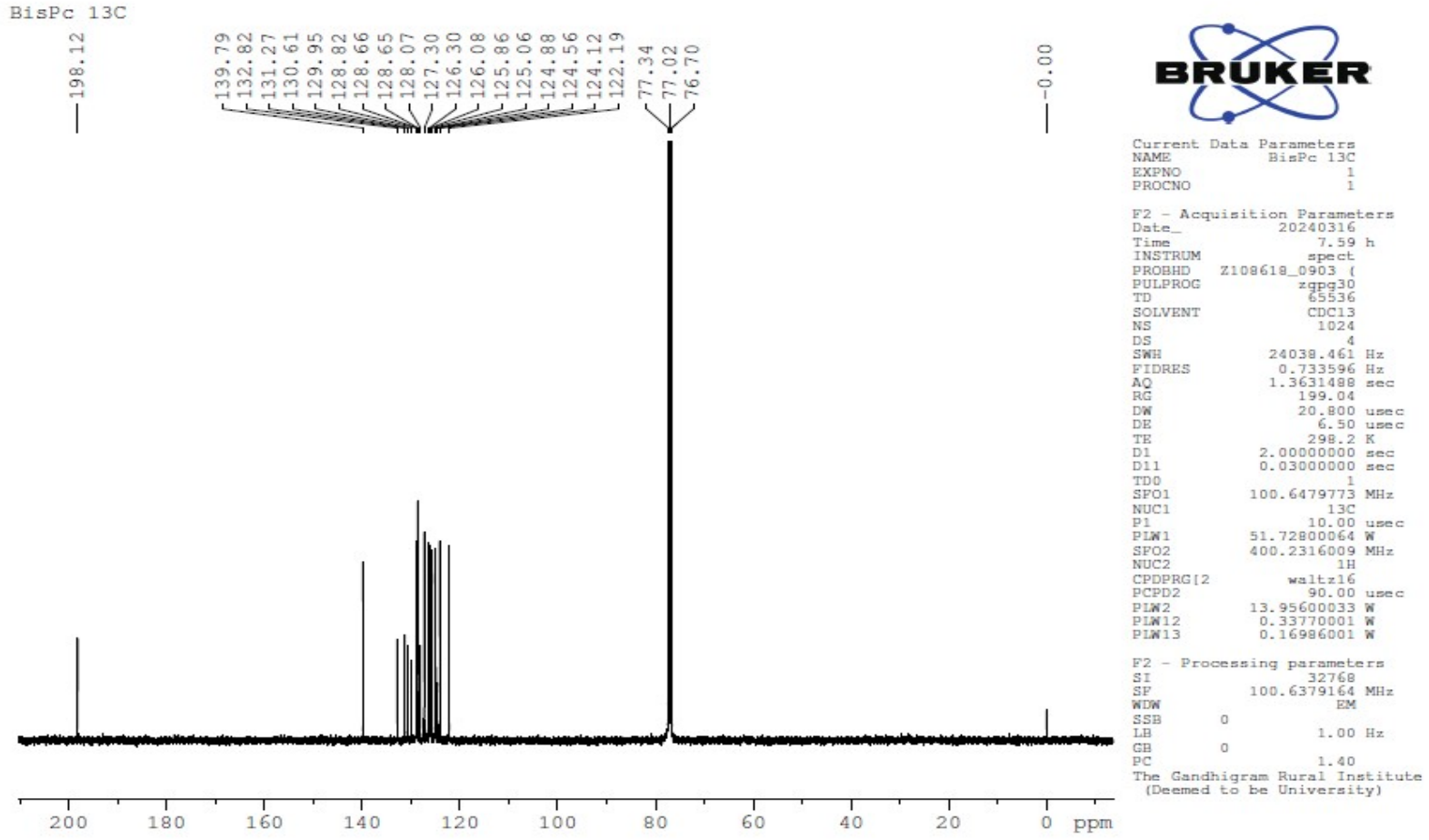

Figure S7c. ^{13}C NMR spectra of (1*E*,4*E*)-1-(4,6-dihydropyren-2-yl)-5-(pyren-4-yl) penta-1,4-dien-3-one (13)