

Supplementary information

Synthesis of trinuclear Zinc(II) cluster composed of [4.4.3.0^{1,5}]tridecane cages: A rapid detection and degradation probe for chemical warfare agent simulant diethyl cyanophosphonate in protein-rich food products

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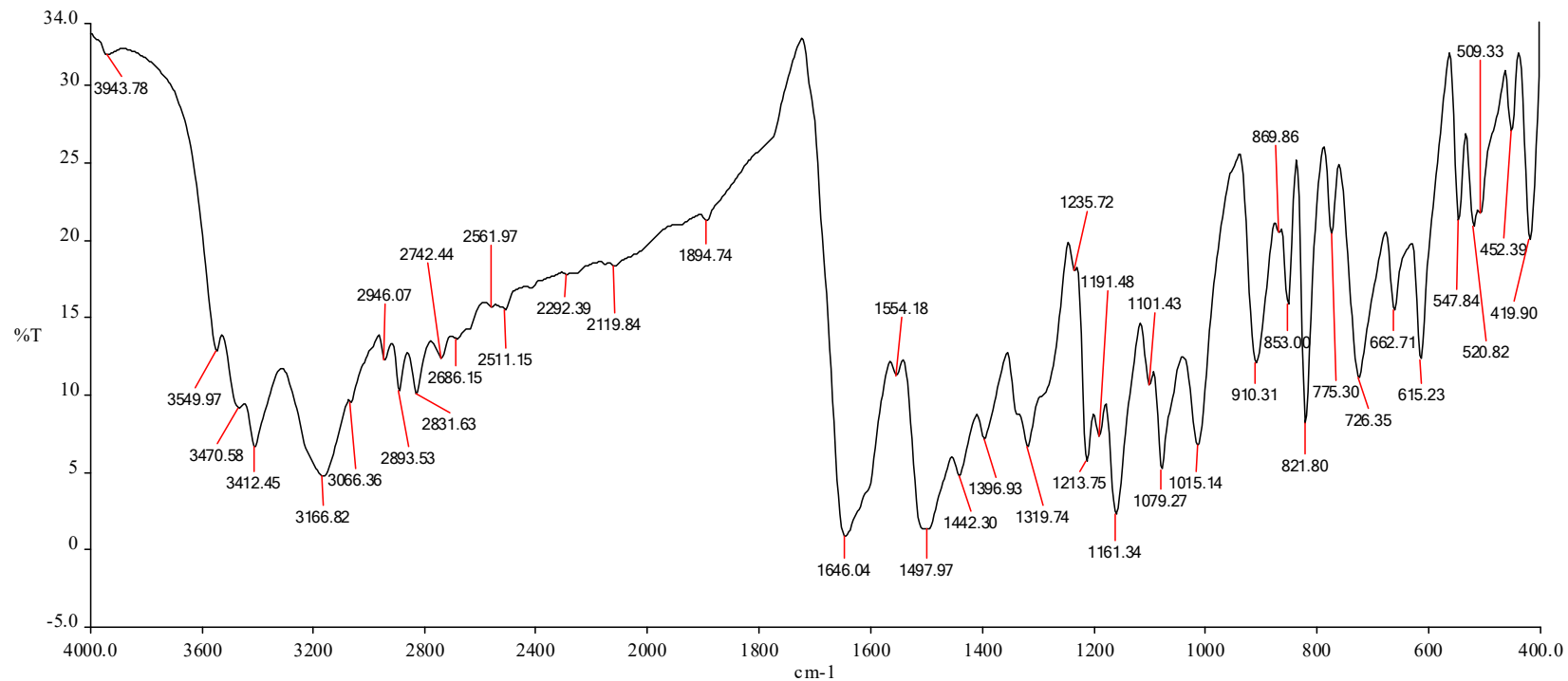
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ES.1 Synthesis of Schiff base (SB)

In a single-neck round bottom flask, ethanolamine (24.55 mmol, 1.50 g) was added to 5-bromosalicylaldehyde (24.55 mmol, 4.93 g) dissolved in 100 mL methanol. The reaction mixture was heated to reflux for 24 h and the contents were cooled to room temperature. The solvent was removed under a vacuum to afford a yellow solid. The product was filtered, washed with hexane and diethyl ether to remove the impurities, dried and stored under dry conditions. Yield: 90.80% (22.24 mmol, 5.43 g), Melting point: 90-92°C; FT-IR (KBr) cm^{-1} : 3300-2950 (br, OH, intramolecular hydrogen-bonded), 1646 (C=N), 1497(C-C), 1079, 1015 (C-O), 726 (C-Br). $^1\text{H-NMR}$ (500 MHz, CDCl_3): δ (ppm) 1.63 (1H, s, Alk-OH), 3.69 (2H, t, $^3J = 5.0$ Hz, H⁹), 3.85 (2H, t, $^3J = 5.0$ Hz, H⁸), 6.78 (1H, d, $^3J = 8.5$ Hz, H²), 7.30 (2H, dd, H³), 7.32 (2H, d, H⁵), 8.24 (1H, s, H⁷), 13.22 (1H, s, Ar-OH); $^{13}\text{C NMR}$ (125 MHz, CDCl_3): δ (ppm) 61.6 (C⁹), 61.9 (C⁸), 110.1 (C⁴), 119.1 (C²), 120.0 (C⁶), 133.6 (C⁵), 135.1 (C³), 160.3 (C⁷), 165.7 (C¹); ESI-MS (m/z): 244.36 (M+H)⁺, 246.36 (M+2+H)⁺. Anal. Calcd for $\text{C}_9\text{H}_{10}\text{NO}_2\text{Br}$ C, 44.29; H, 4.13; N, 5.74; Found: C, 44.28; H, 4.12; N, 5.76.



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Figure S1 FT-IR spectrum of Schiff base (SB)

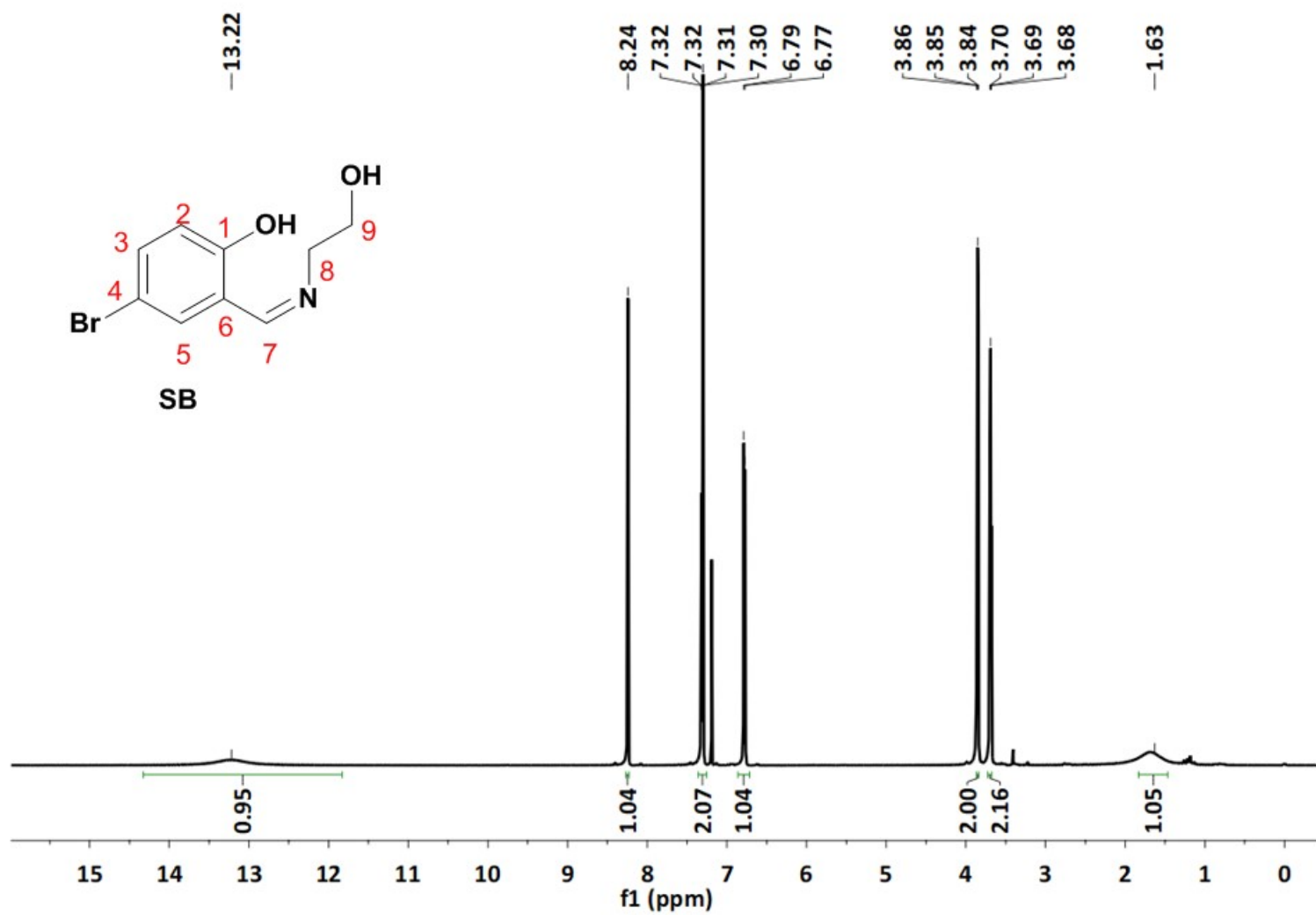


Figure S2 ¹H-NMR spectrum (500 MHz, CDCl₃) Schiff Base (SB).

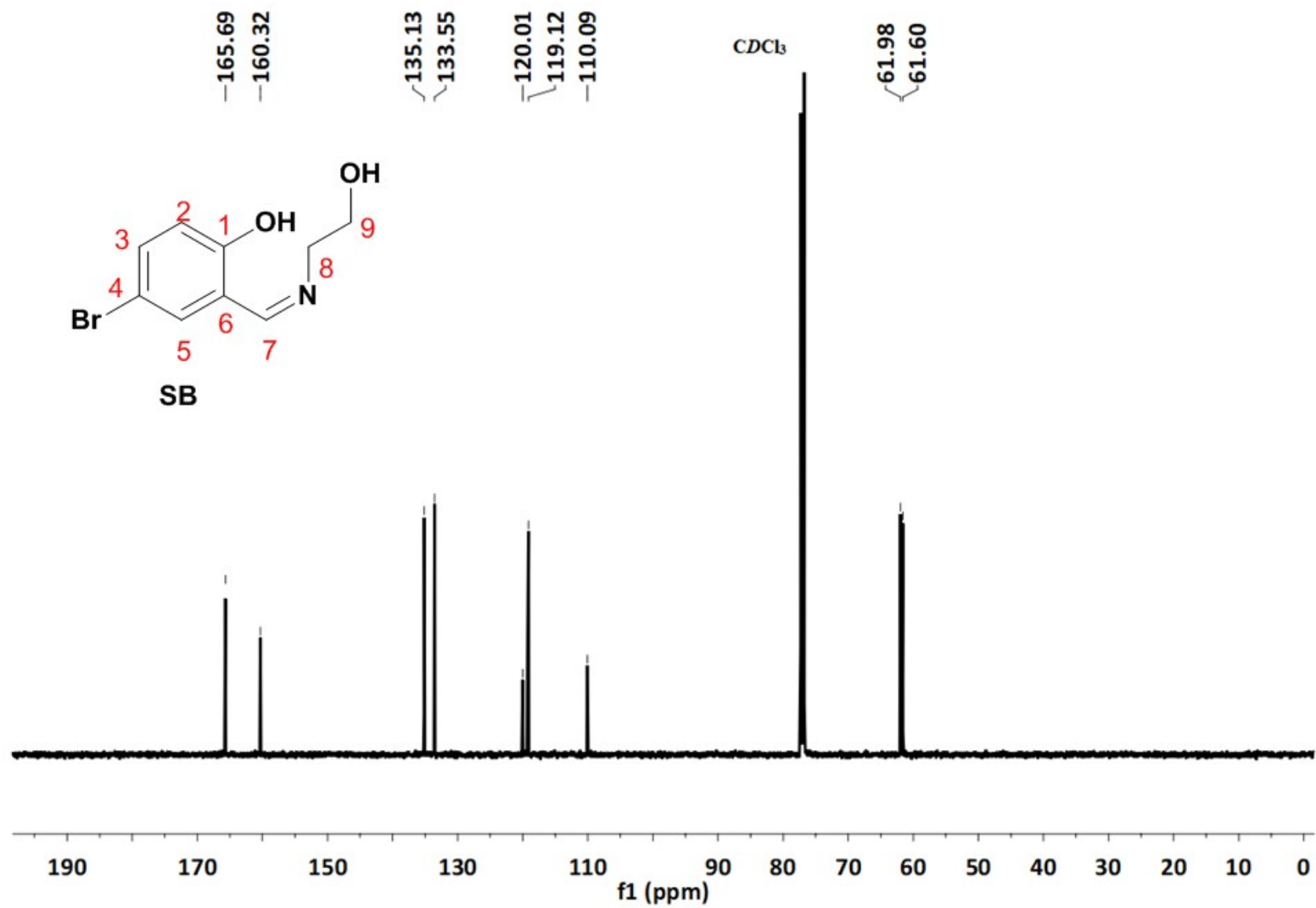


Figure S3 ¹³C-NMR spectrum (125 MHz, CDCl₃) Schiff Base (SB).

WATERS,Q-TOF MICROMASS (ESI-MS)

JYOTI SB 35 (0.533) Sm (SG, 2x3.00); Cm (16:47)

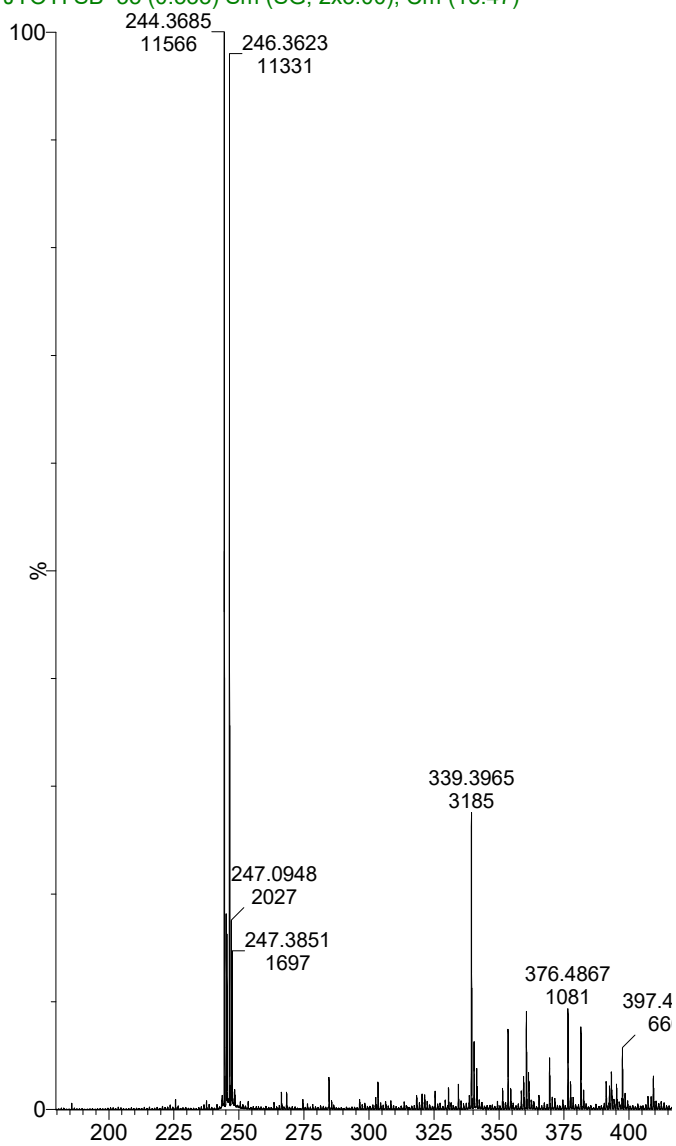
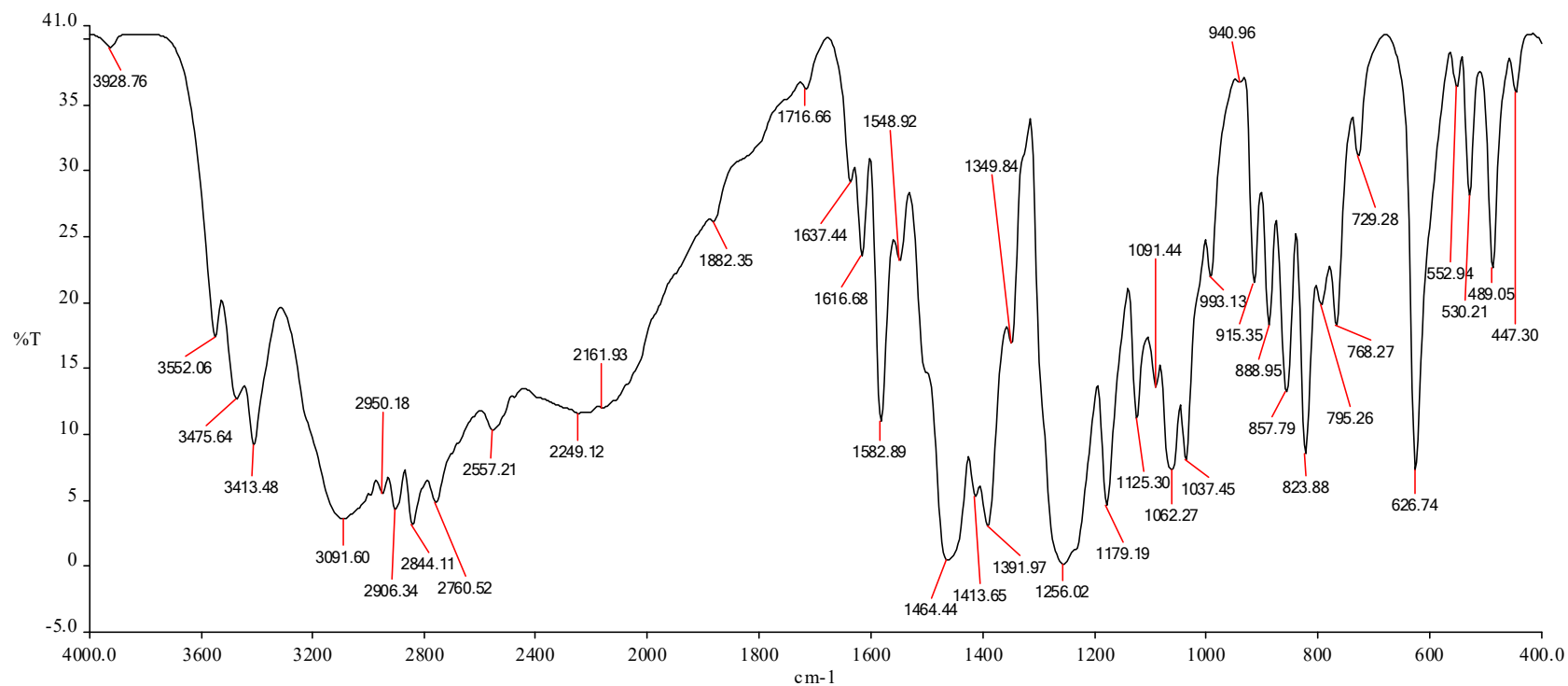


Figure S4 ESI-MS spectrum of Schiff base (SB).



ROHILLA JYOTI 3.asc - 01/18/2022 - RSB IR

Figure S5 FT-IR spectrum of reduced Schiff base (rSB)

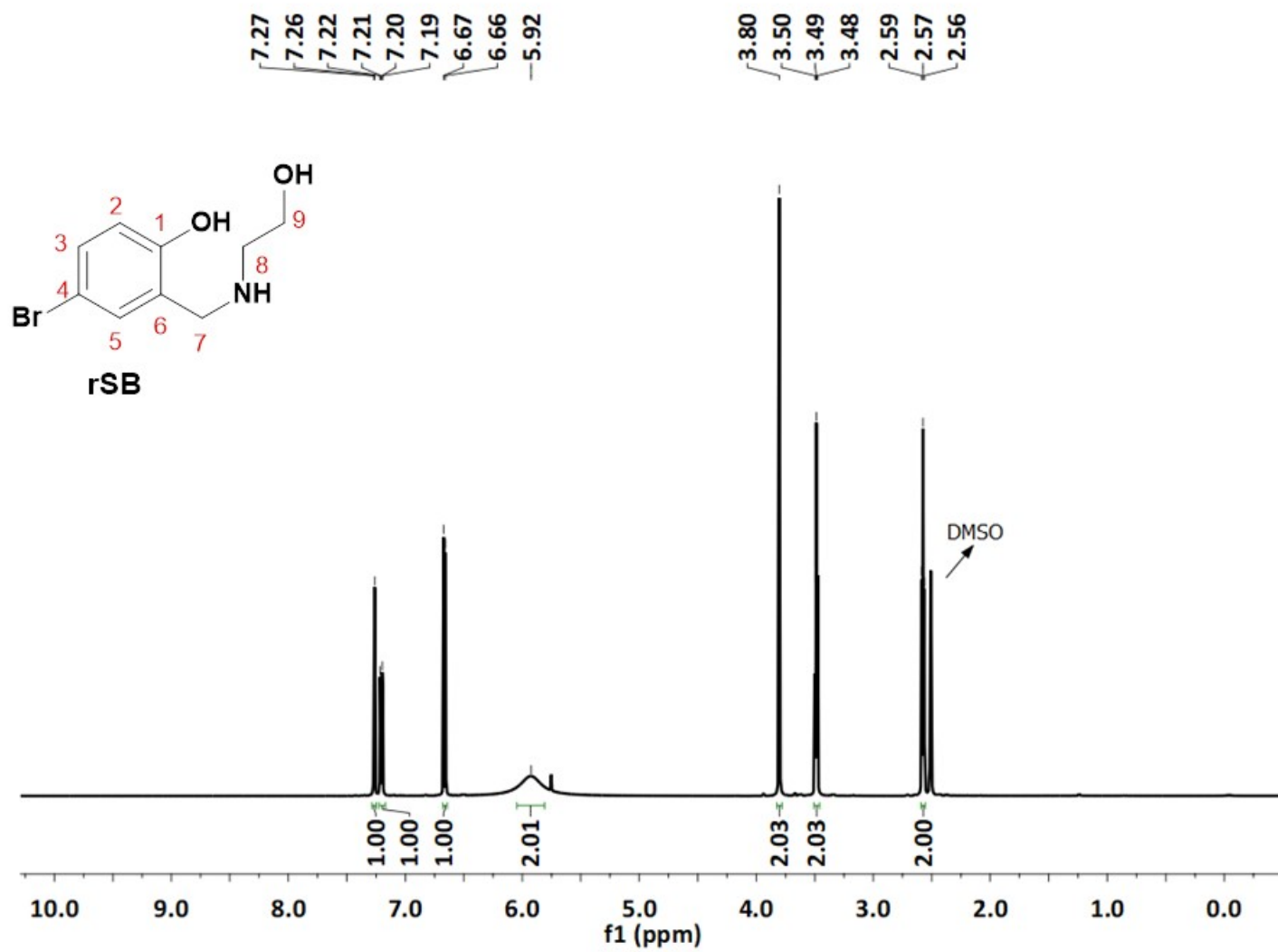


Figure S6 ¹H-NMR spectrum (500 MHz, DMSO) of reduced Schiff Base (rSB).

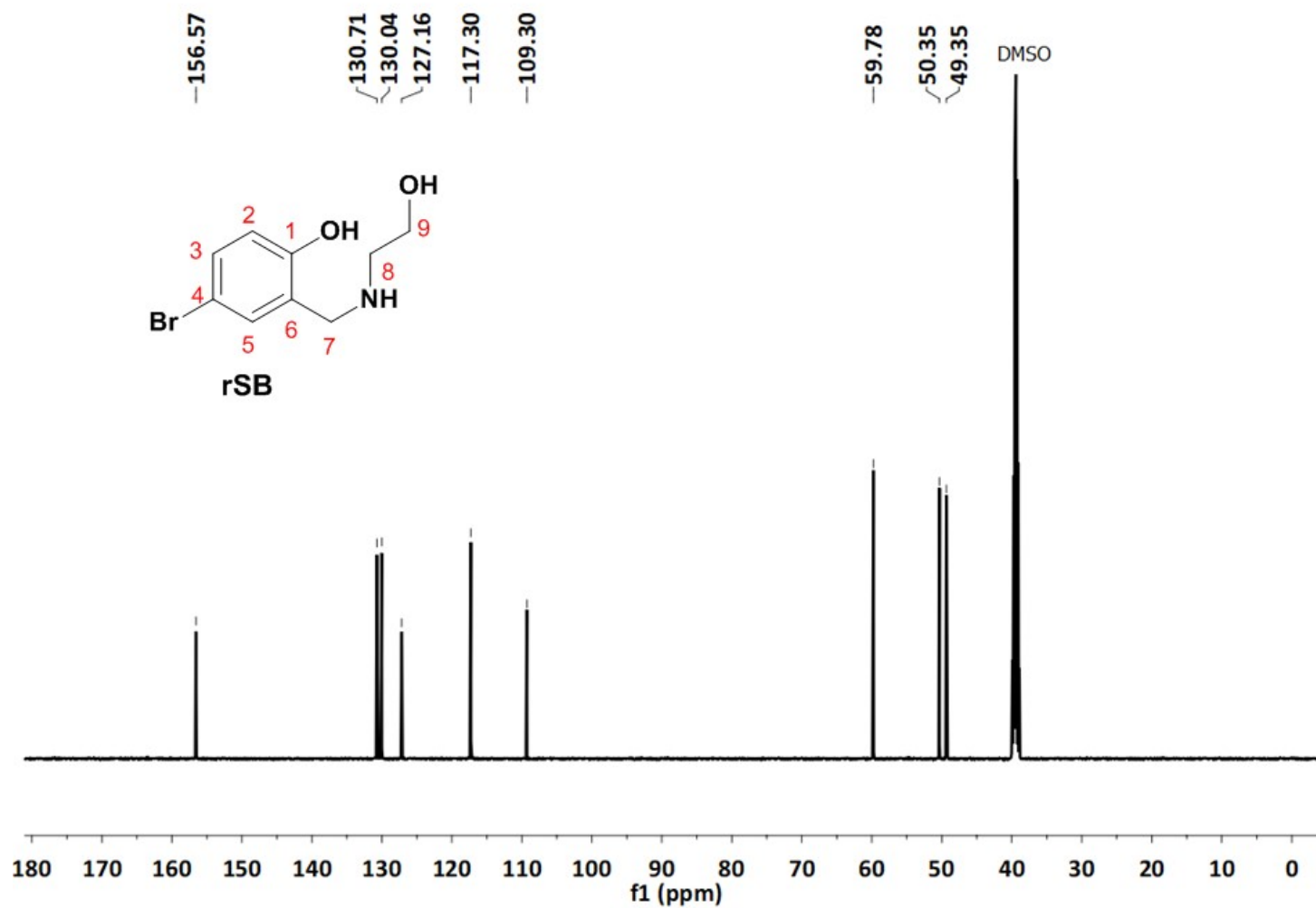


Figure S7 ¹³C-NMR spectrum (125 MHz, DMSO) of reduced Schiff Base (rSB).

WATERS, Q-TOF MICROMASS (ESI-MS)

JYOTI RSB 40 (0.608) Sm (SG, 2x3.00); Cm (31:50)

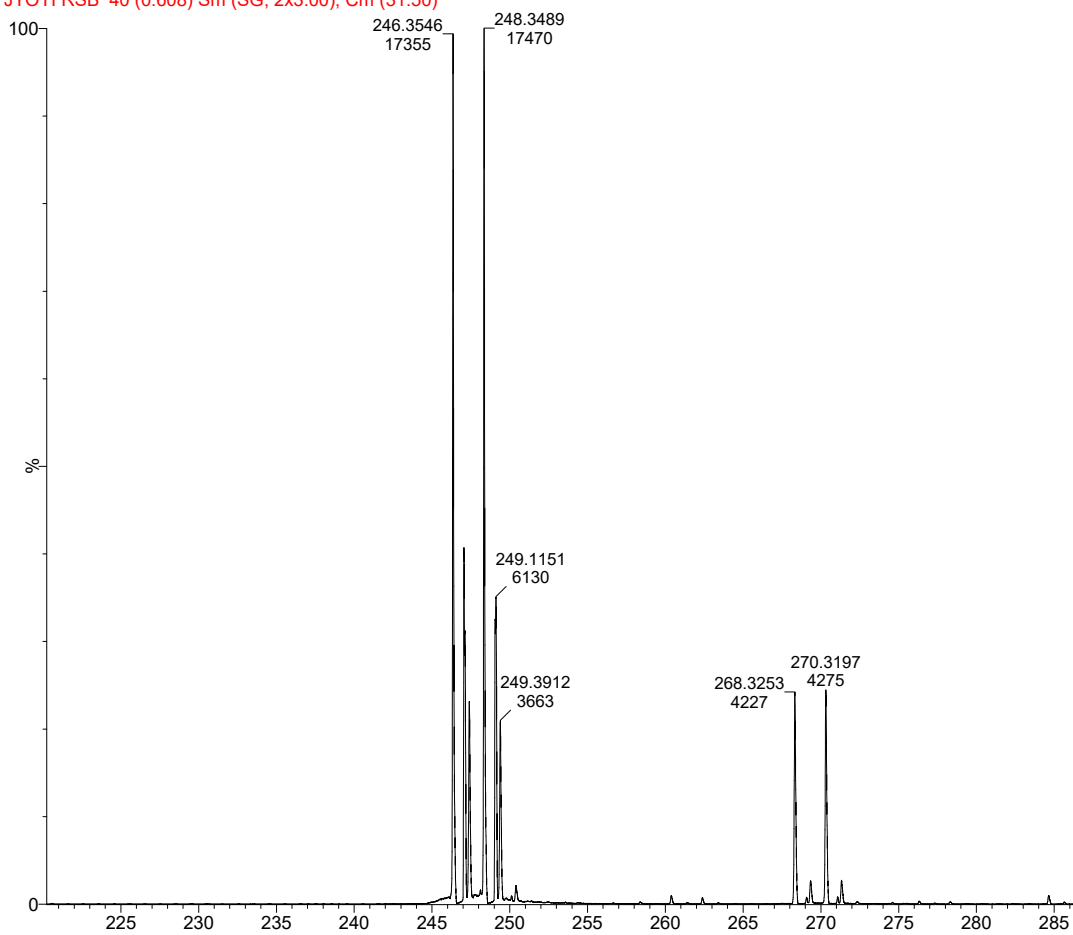


Figure S8 ESI-MS spectrum of reduced Schiff Base (rSB).

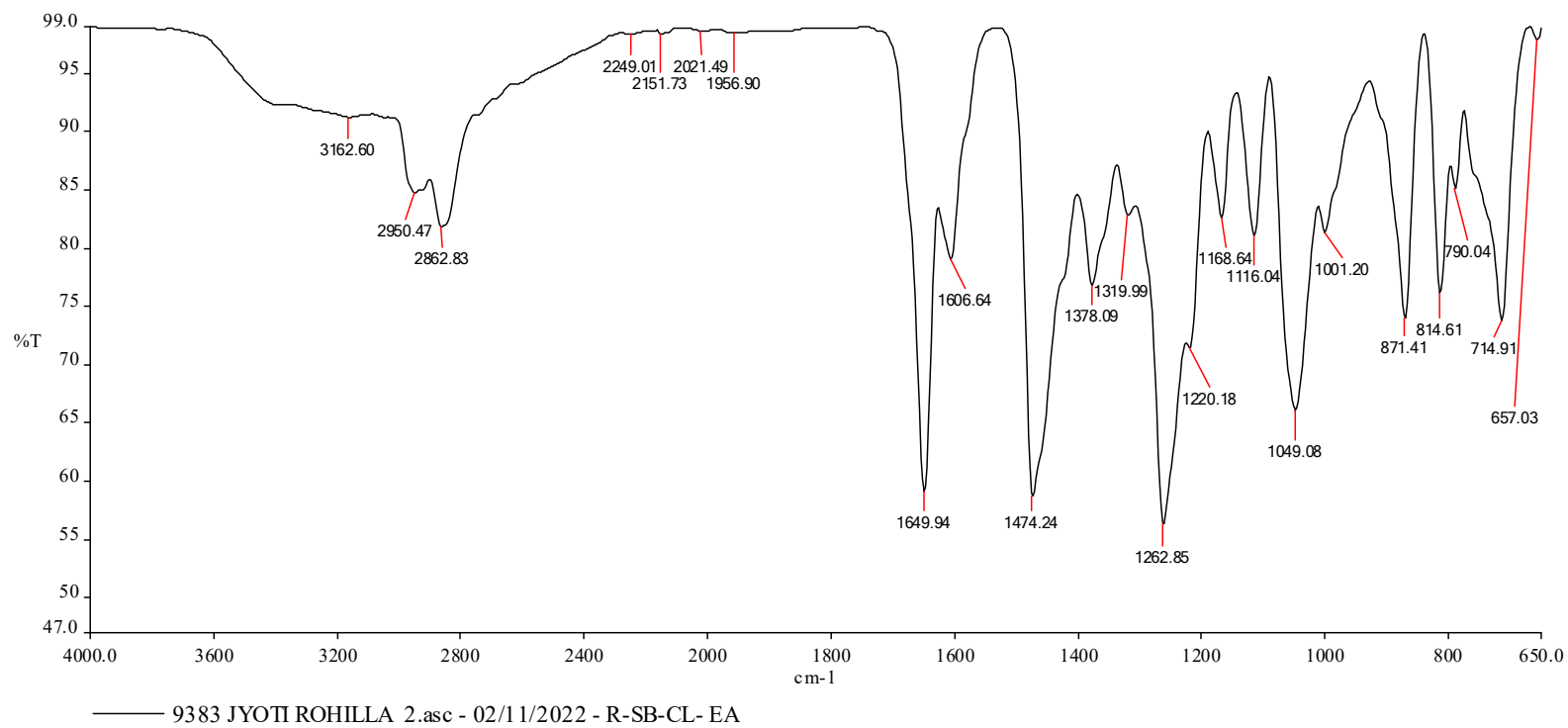


Figure S9 FT-IR spectrum of tripodal amine (TPA).

Fig

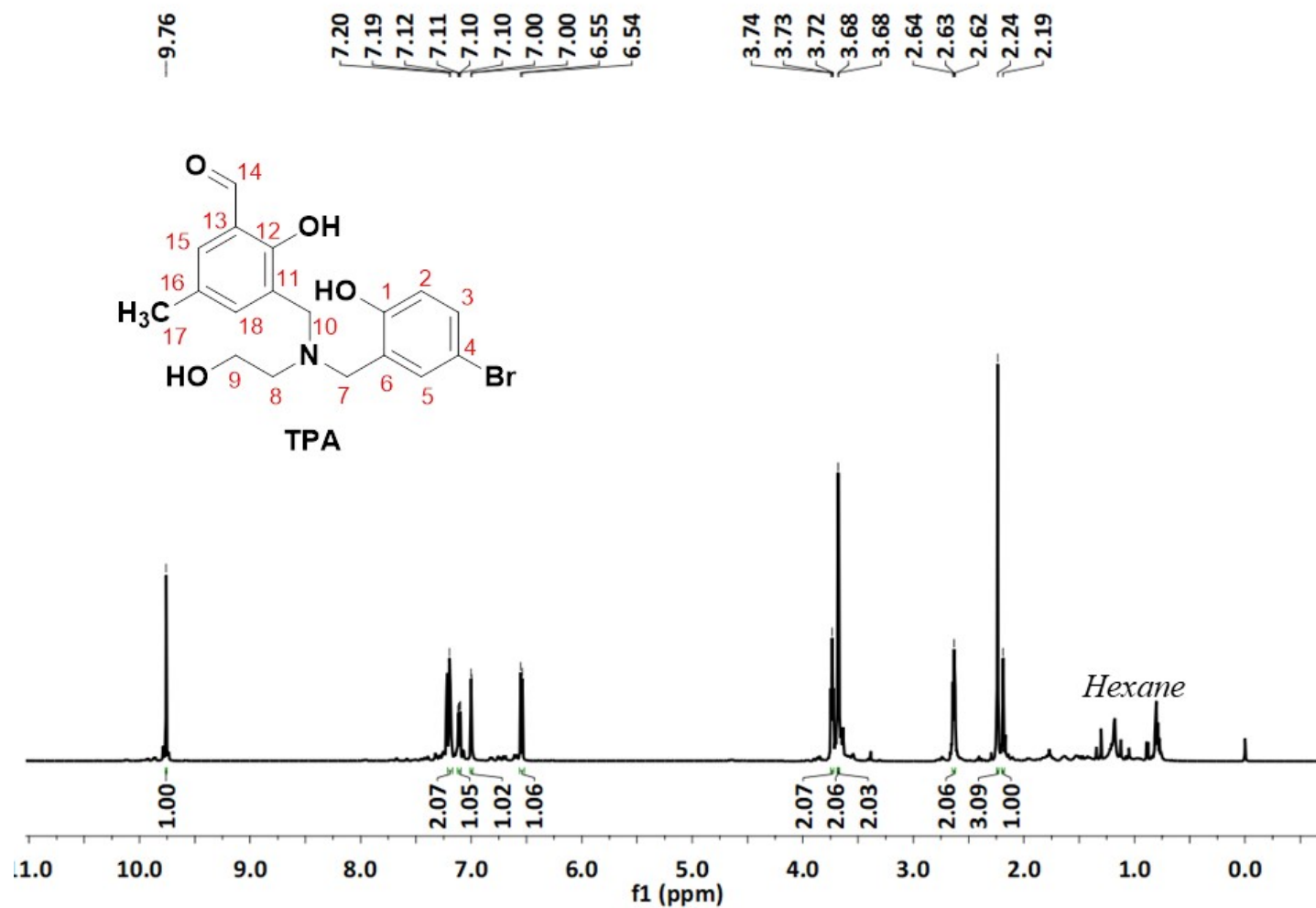


Figure S10 ¹H-NMR spectrum (500 MHz, CDCl₃) of tripodal amine (TPA).

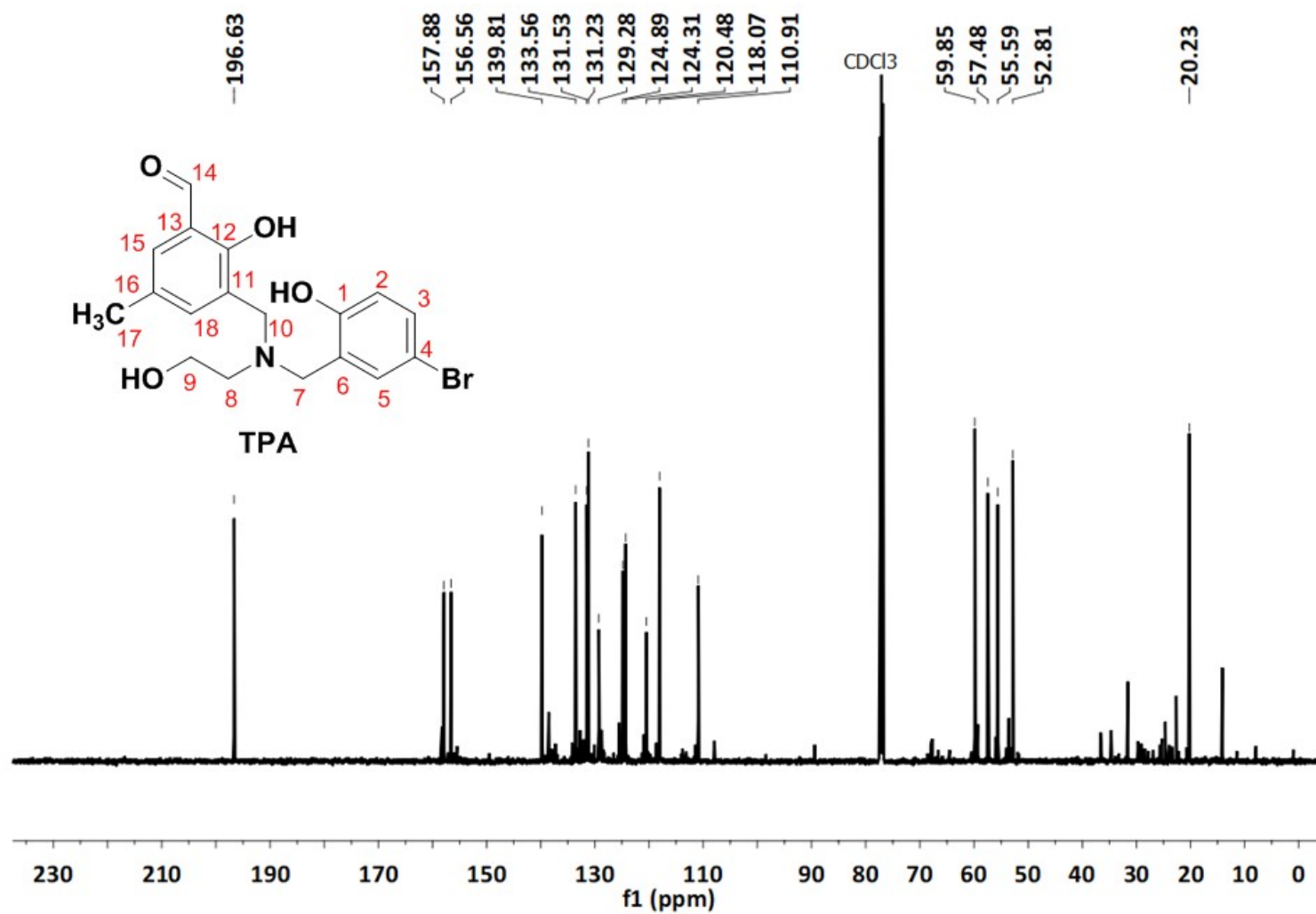


Figure S11 ¹³C-NMR spectrum (125 MHz, CDCl₃) of tripodal amine (TPA).

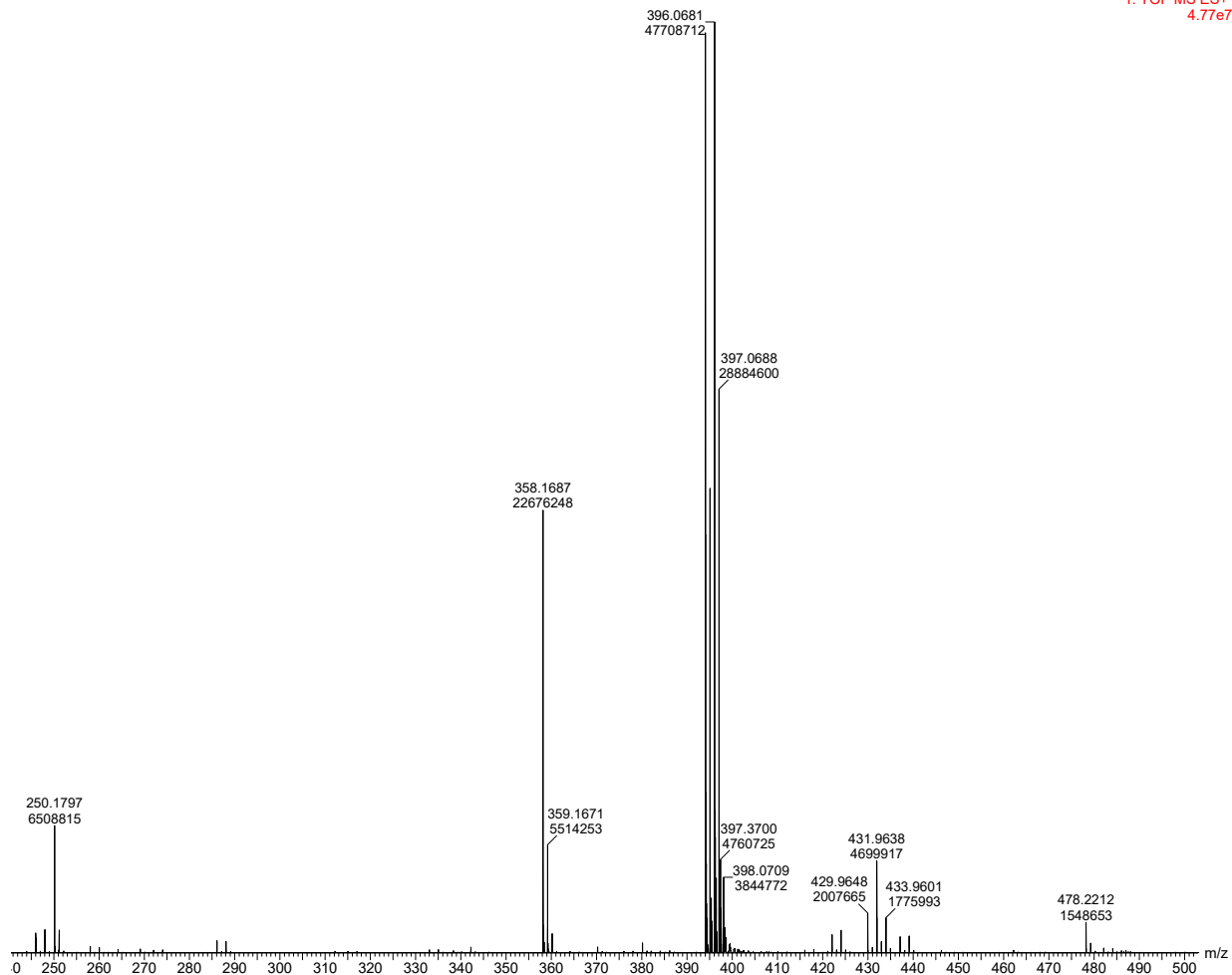


Figure S12 ESI-MS spectrum of tripodal amine (TPA).

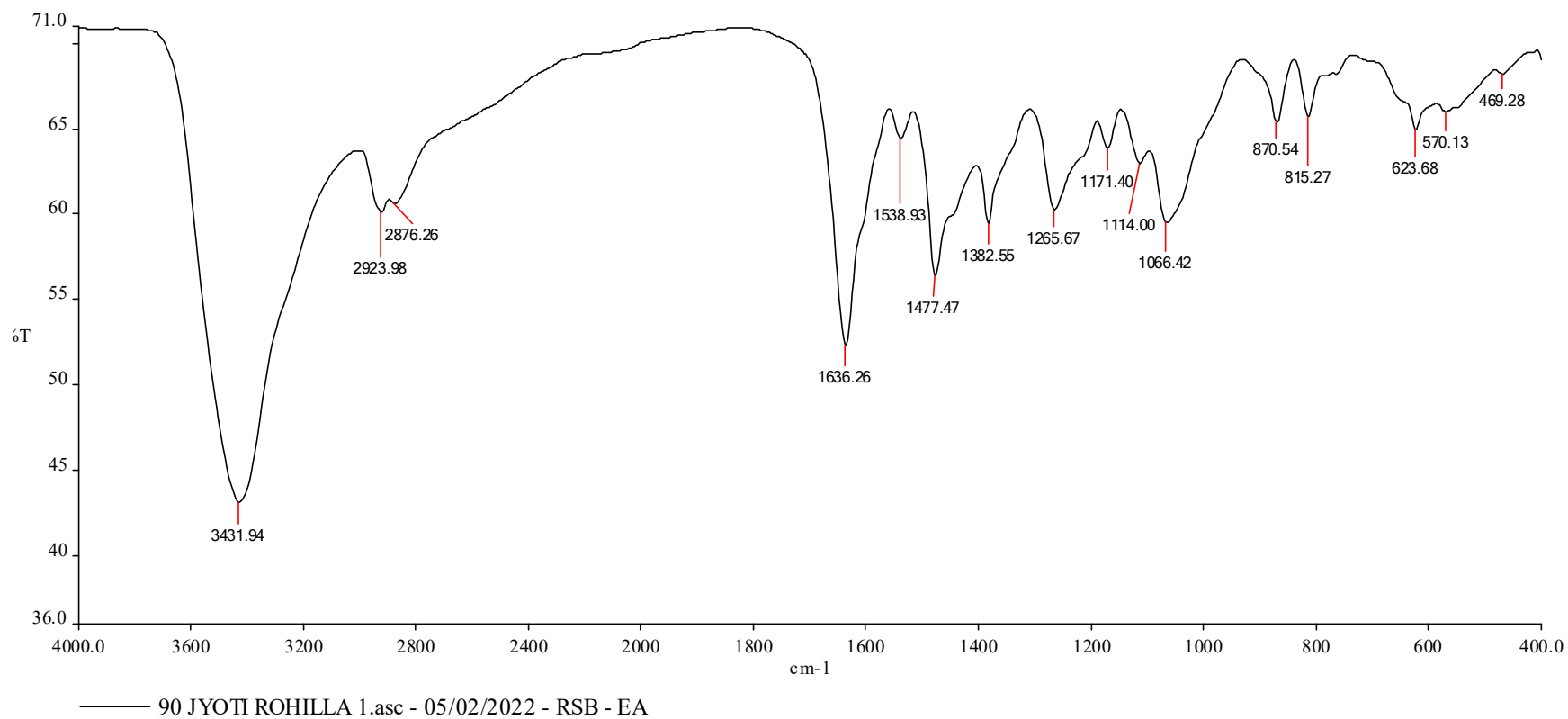


Figure S13 FT-IR spectrum of compartmental ligand H₃L

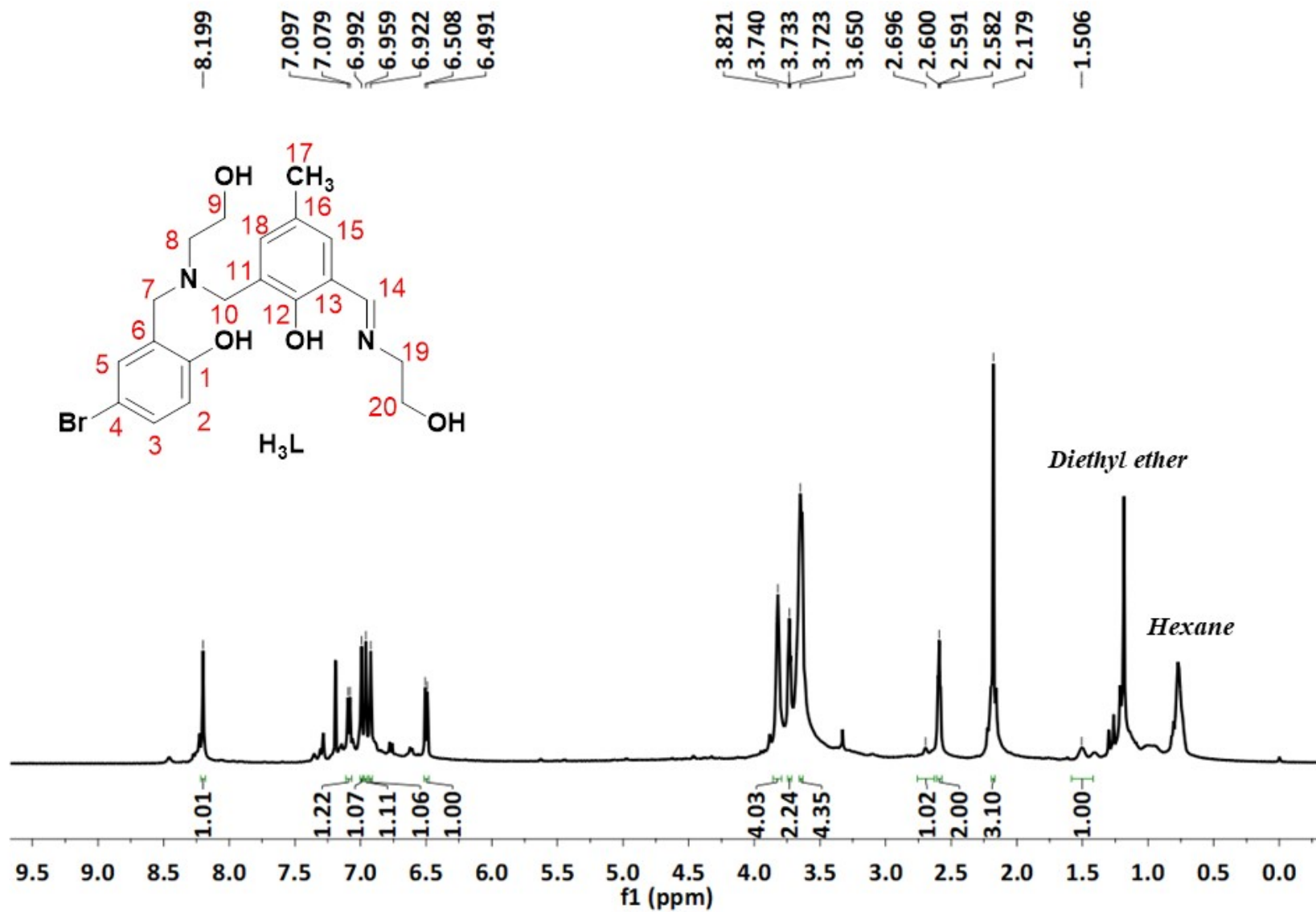


Figure S14 1H -NMR spectrum (500 MHz, $CDCl_3$) of compartmental ligand H_3L

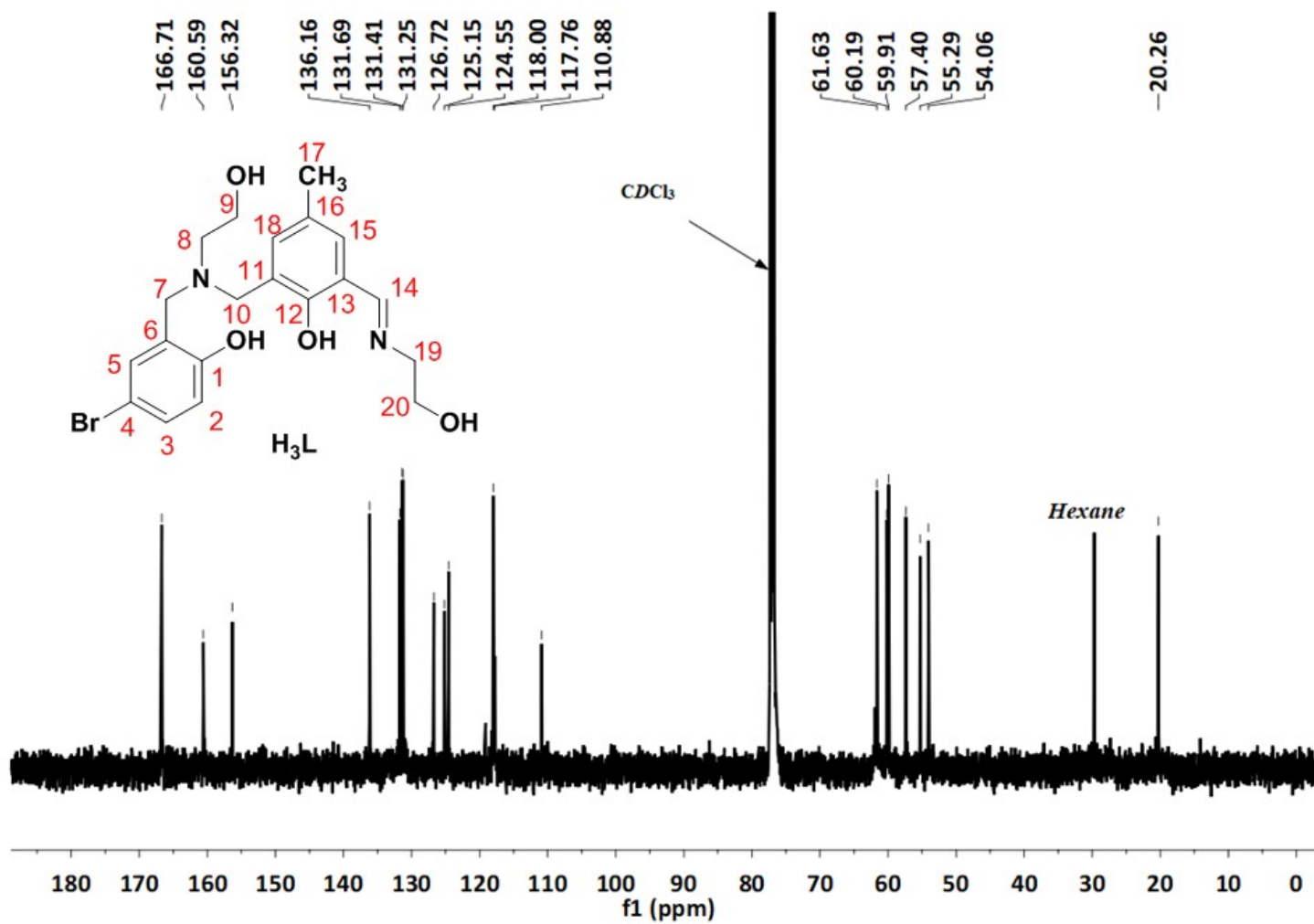


Figure S15 ^{13}C -NMR spectrum (125 MHz, $CDCl_3$) of compartmental ligand H_3L

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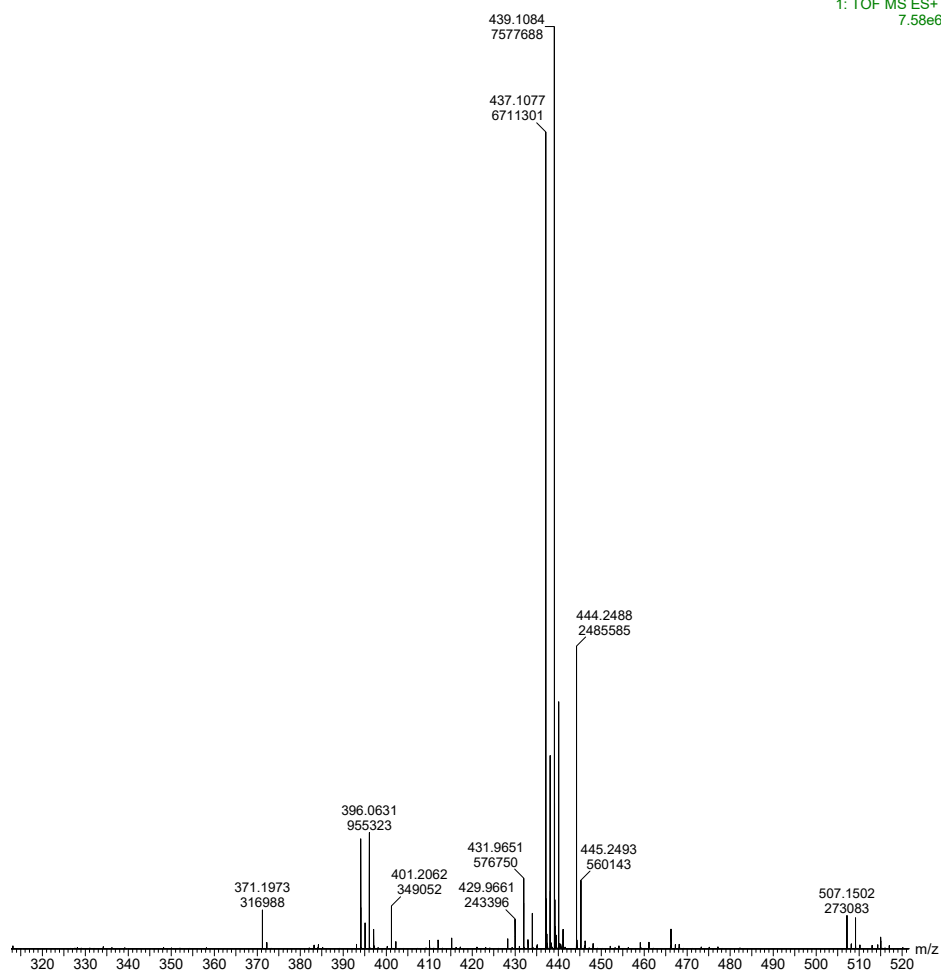


Figure S16 ESI-MS spectrum of ligand H₃L

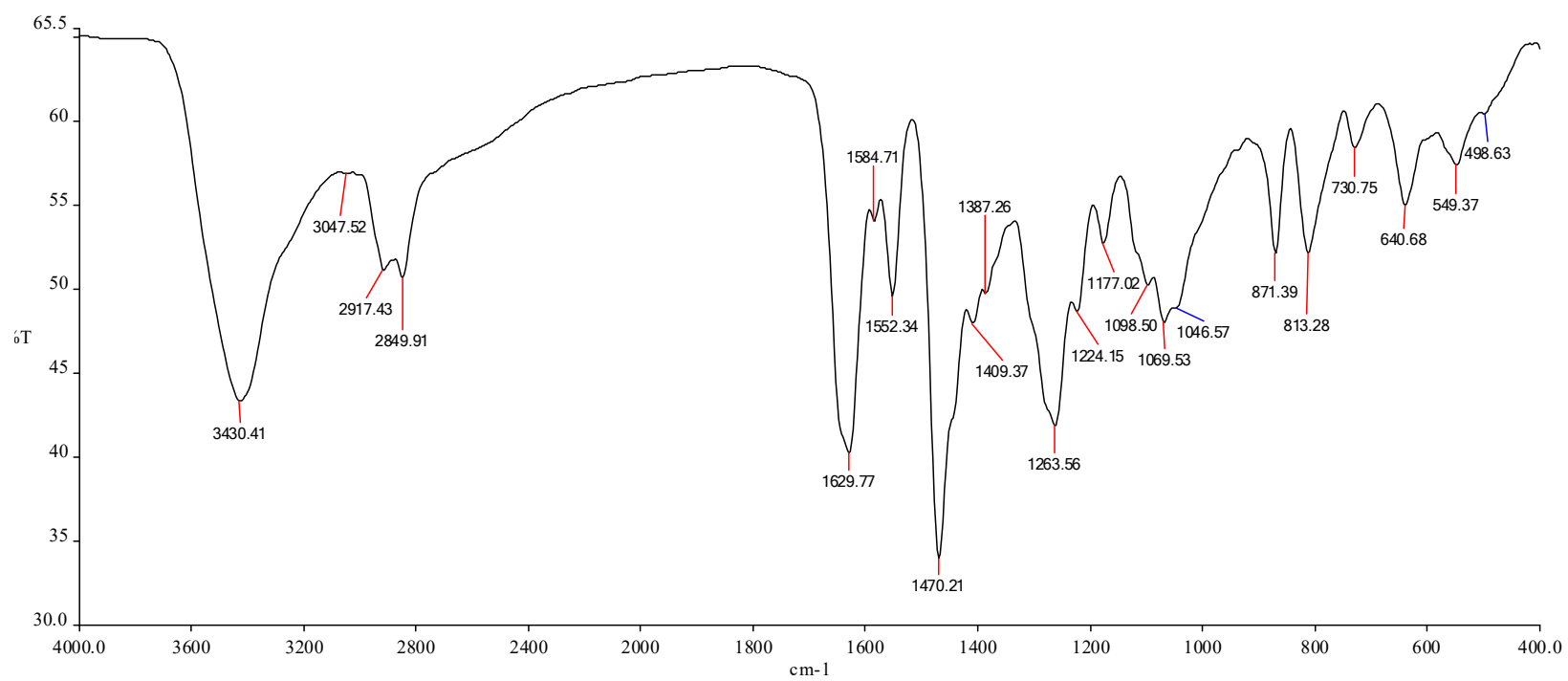


Figure S17 FT-IR spectrum of trinuclear Zinc(II) cluster

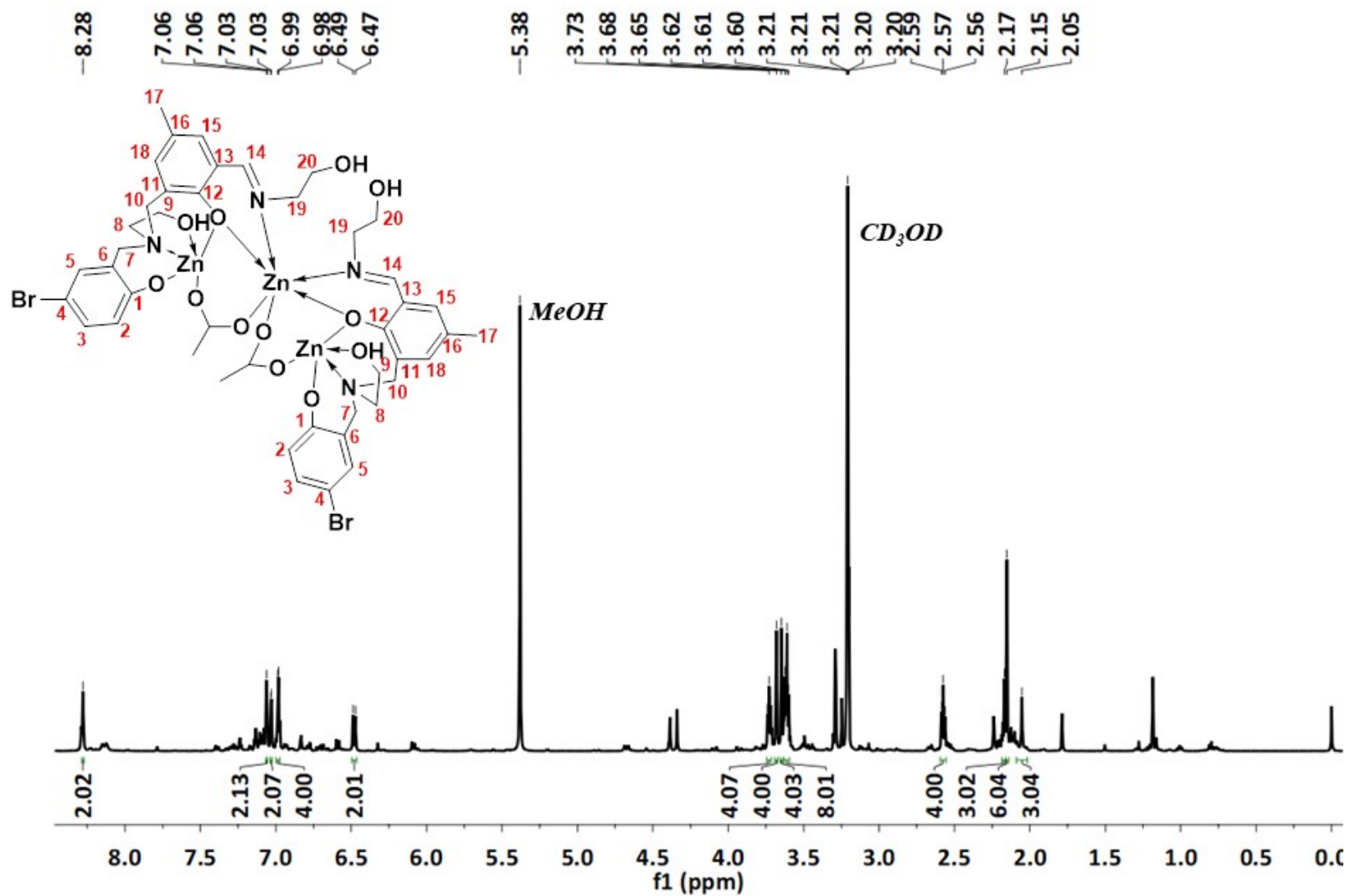


Figure S18 $^1\text{H-NMR}$ spectrum (500 MHz, CD_3OD) of trinuclear Zinc(II) cluster

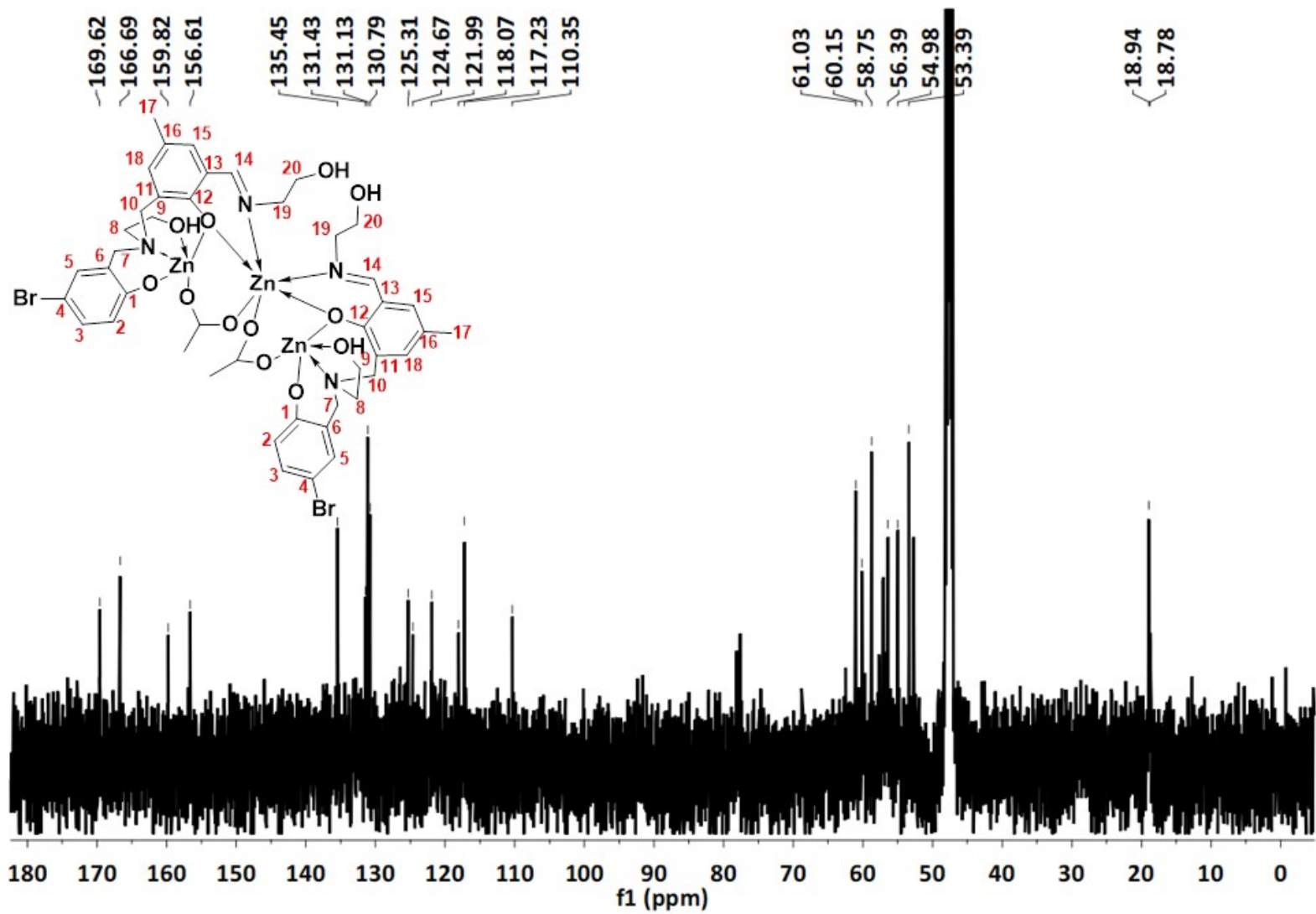


Figure S19 ¹³C-NMR spectrum (125 MHz, CD₃OD) trinuclear Zinc(II) cluster

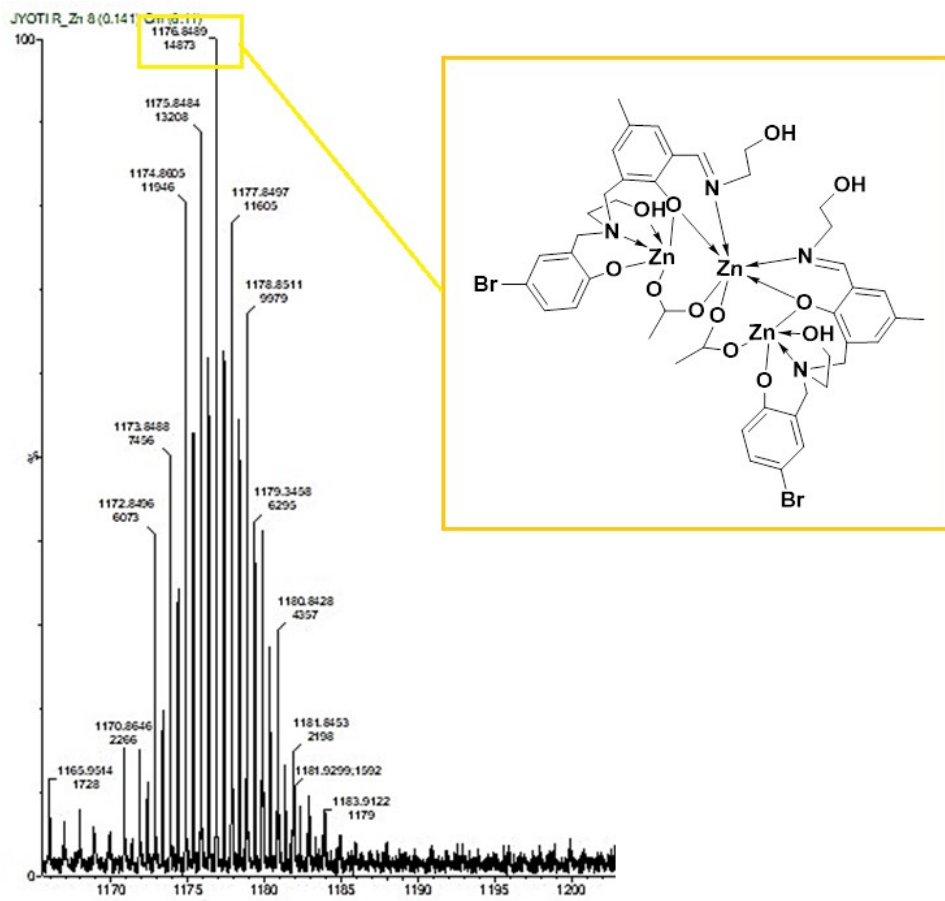


Figure S20 ESI-MS spectrum of trinuclear Zinc(II) cluster

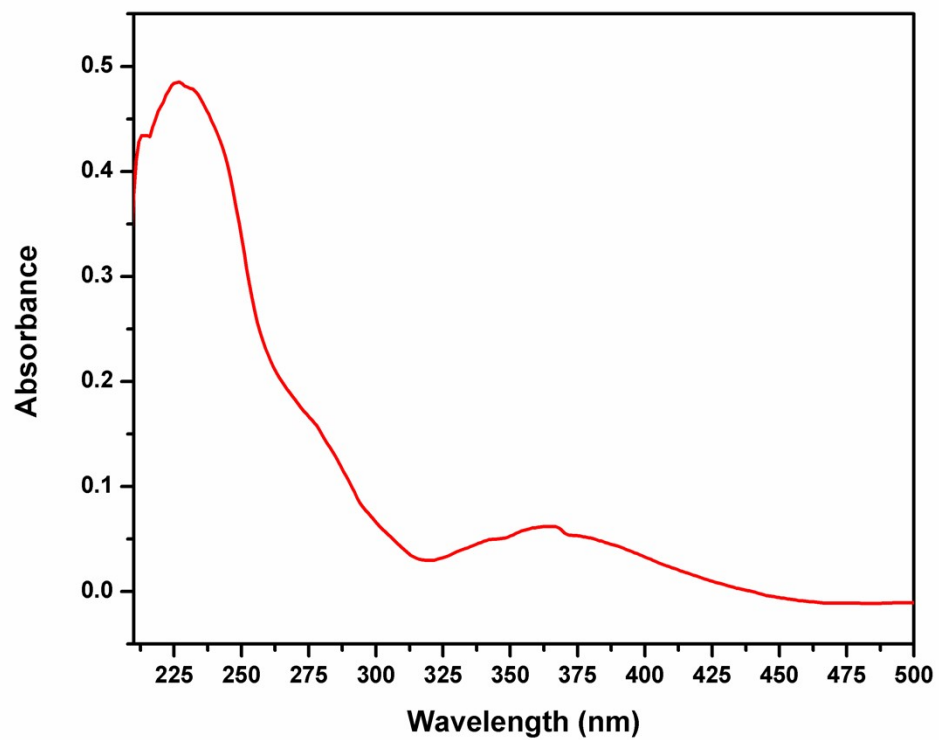


Figure S21 UV-Visible spectrum of trinuclear Zinc(II) cluster

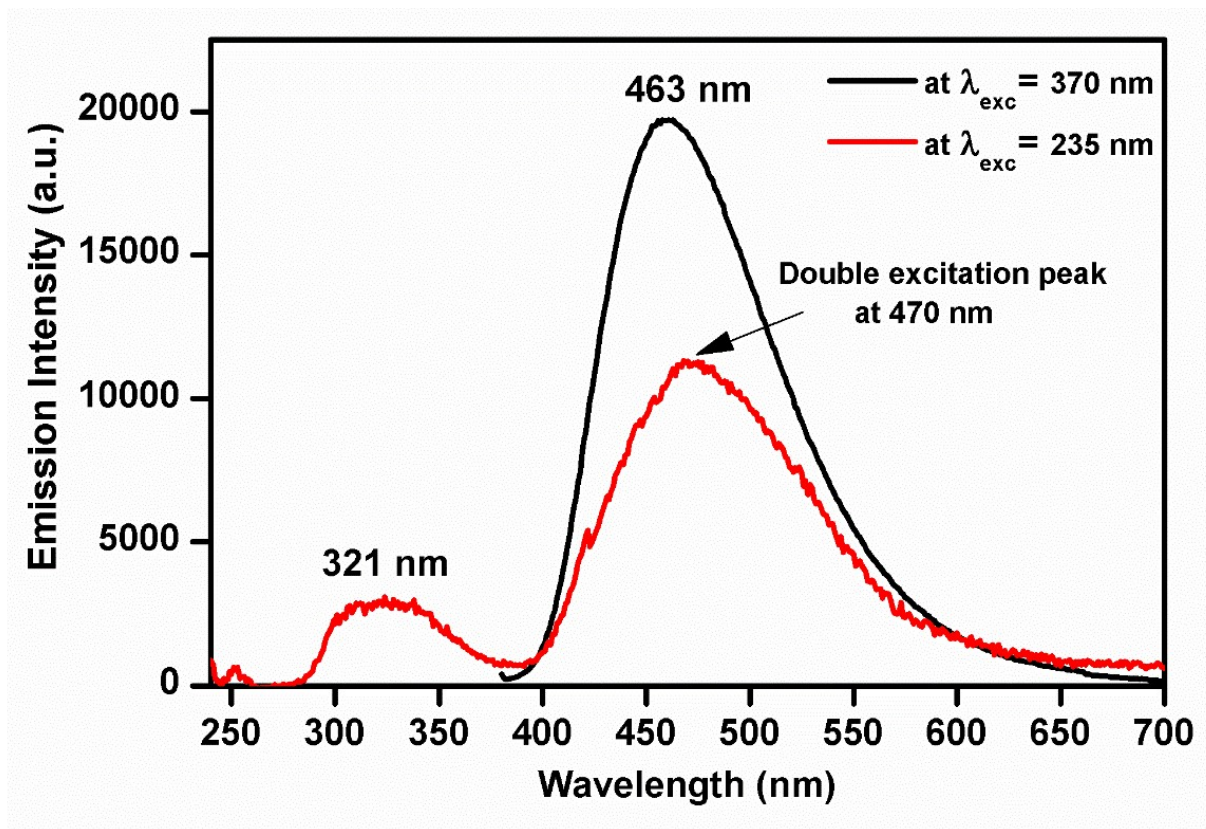


Figure S22 Fluorescence response of the trinuclear Zinc(II) cluster [At $\lambda_{exc} = 235$ nm, it gives a weak band at 321 nm and a double excitation band centred at 470 nm while at $\lambda_{exc} = 370$ nm, it gives a strong intense response at 463 nm in fluorescence emission spectra].

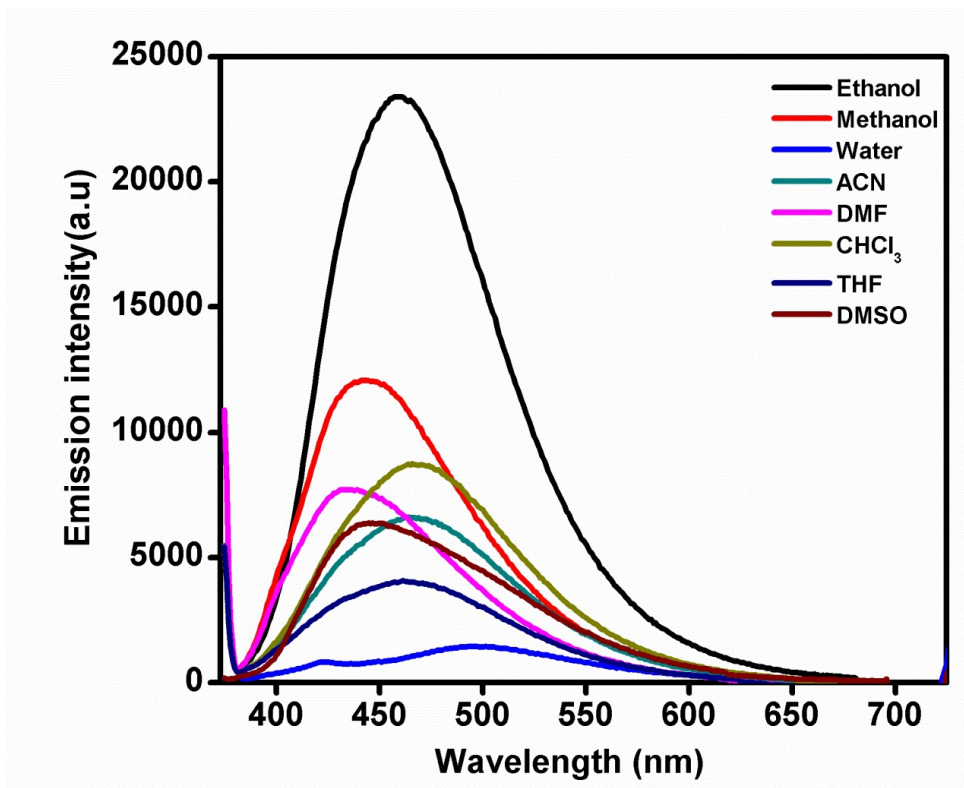


Figure S23 Solvent system optimization: Spectrofluorometric response of trinuclear Zinc(II) cluster in pure solvents (i.e. THF, methanol, ethanol, acetonitrile, chloroform, DMSO, DMF) and water. 2 mL of stock solution of trinuclear Zinc(II) cluster (10 μM) in various solvents mentioned was screened at an excitation wavelength $\lambda_{\text{exc}} = 370$ nm.

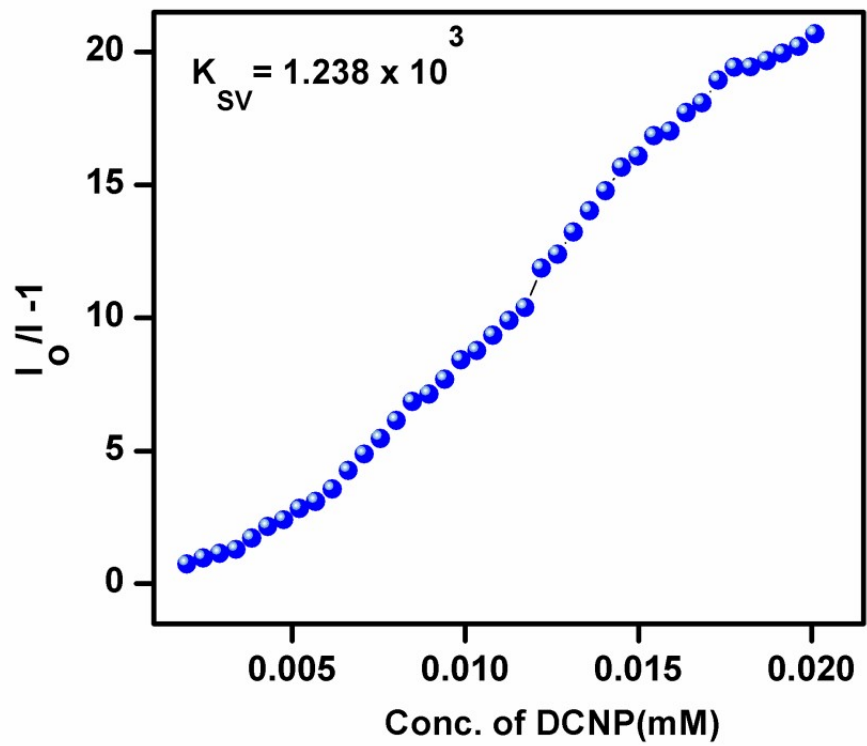


Figure S24 Stern-Volmer plot

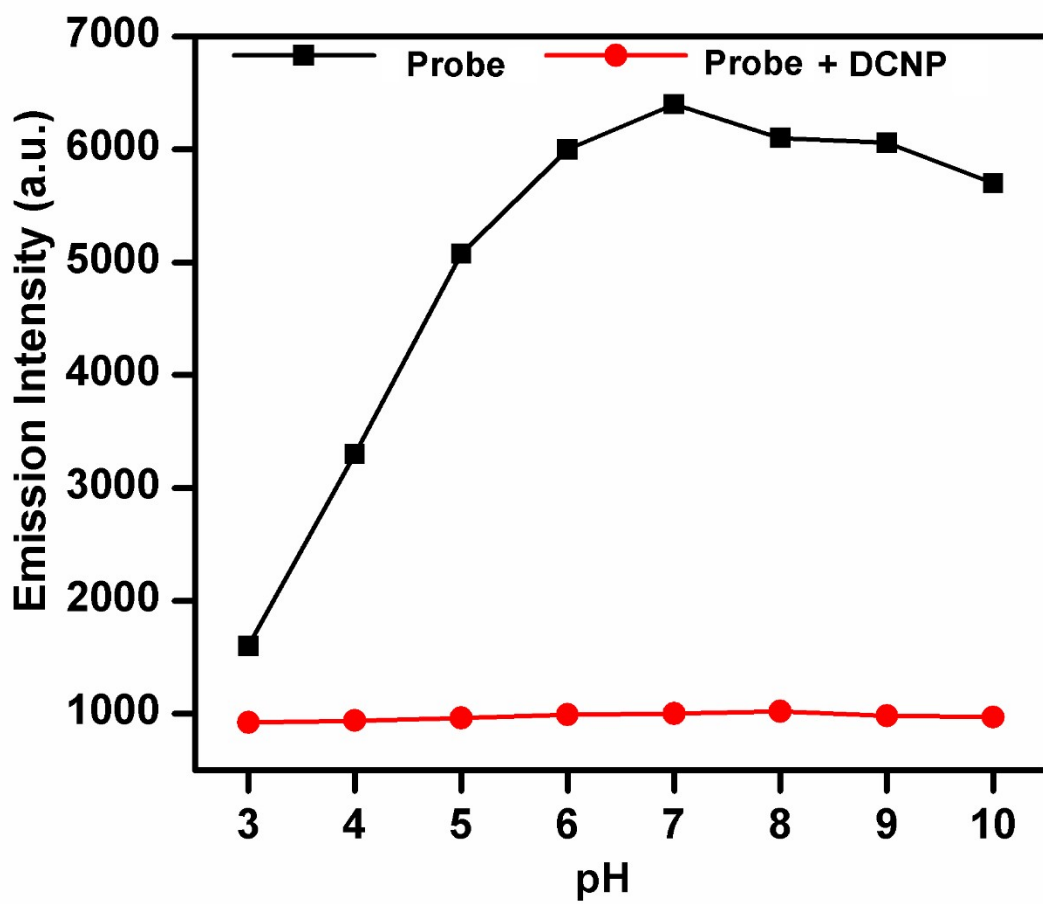


Figure S25 Effect of pH on the fluorescence intensity of trinuclear Zinc(II) cluster and Zinc(II) cluster -DCNP.

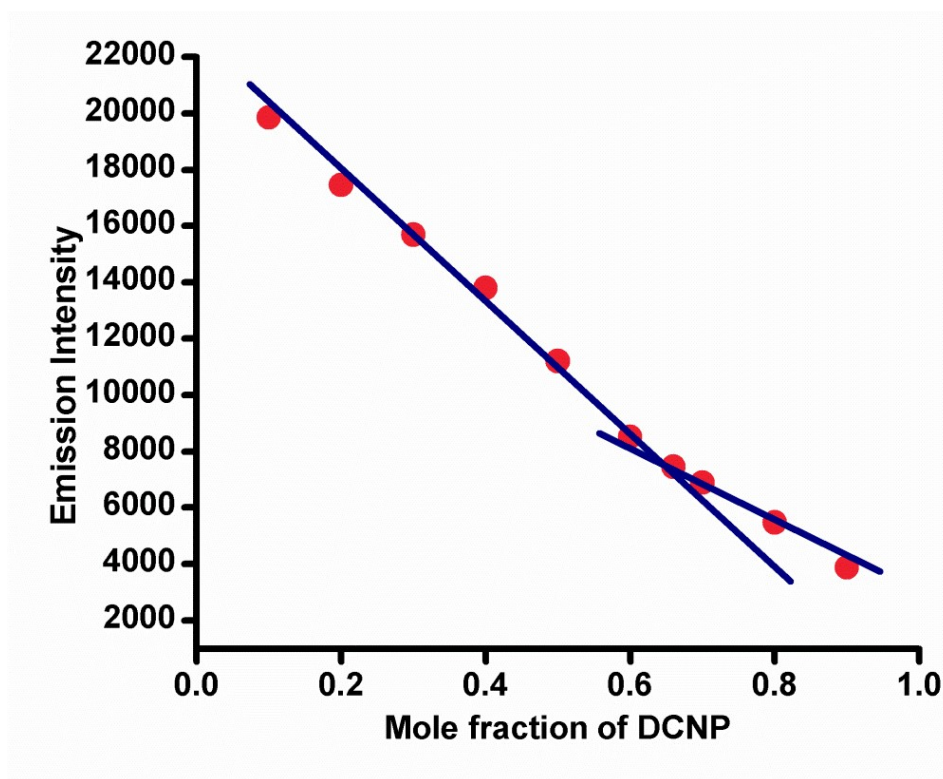


Figure S26 Job plot for the interaction between trinuclear Zinc(II) cluster and DCNP.

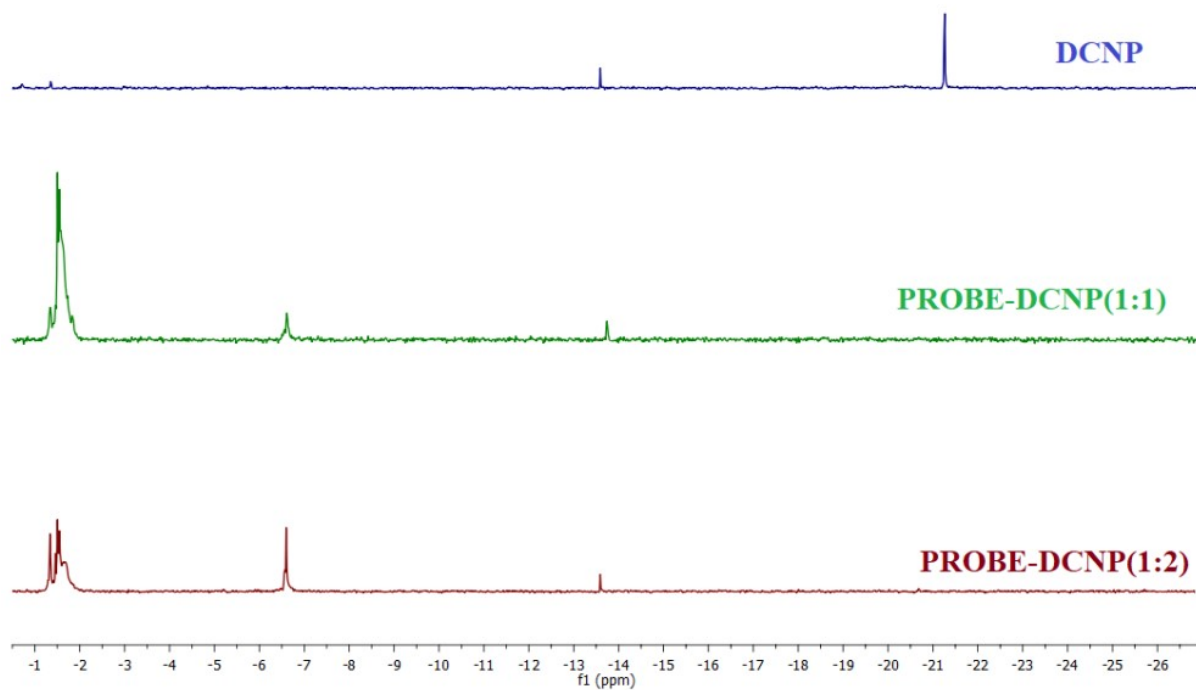


Figure S27 ^{31}P NMR titration of DCNP and trinuclear Zinc(II) cluster (PROBE) in 1:1 and 1:2 stoichiometry in MeOH-d^4 .

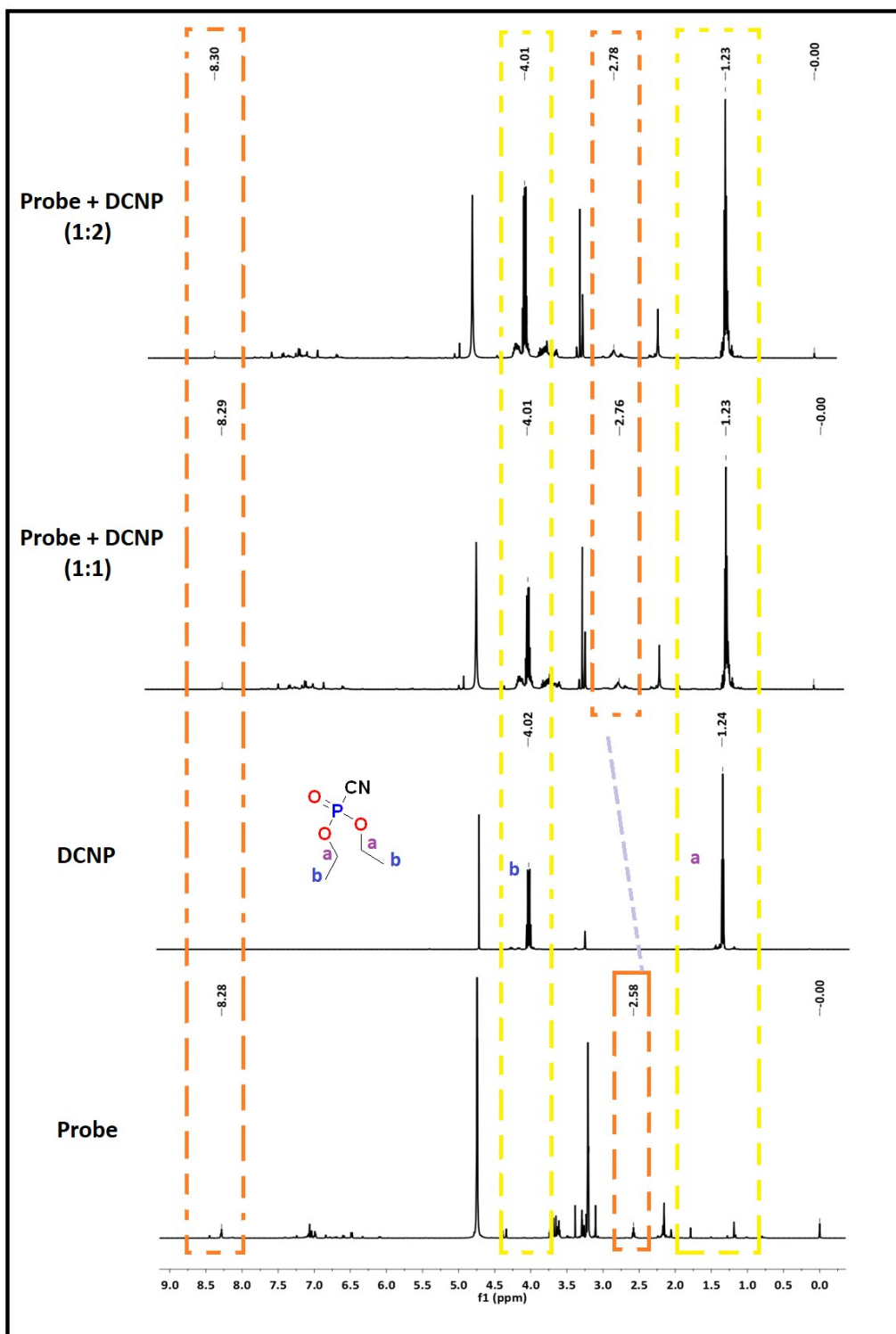


Figure S28 ^1H NMR titration of DCNP and trinuclear Zinc(II) cluster (PROBE) in 1:1 and 1:2 stoichiometry at 500 MHz in MeOH-d^4 .

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JYOTI_ZN_CN 4 (0.103) Cm (4:7)

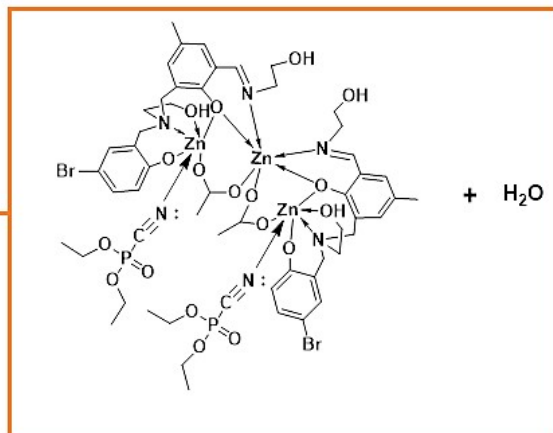
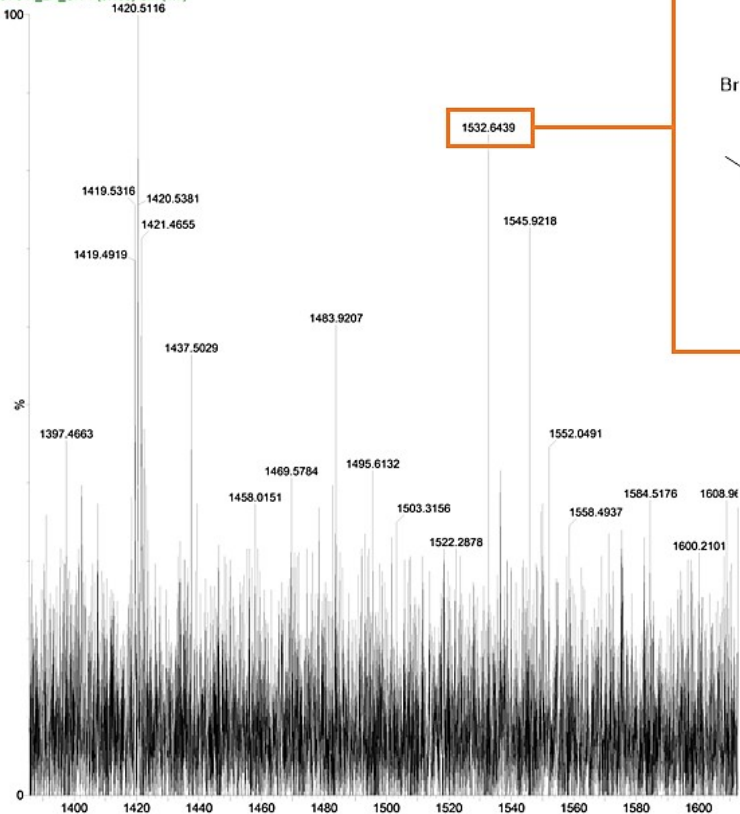


Figure S29 MS (m/z) showing the formation of product formed after the addition of DCNP to trinuclear Zinc(II) cluster

JYOTI_ZN_CN 4 (0.403) Cn (4.7)

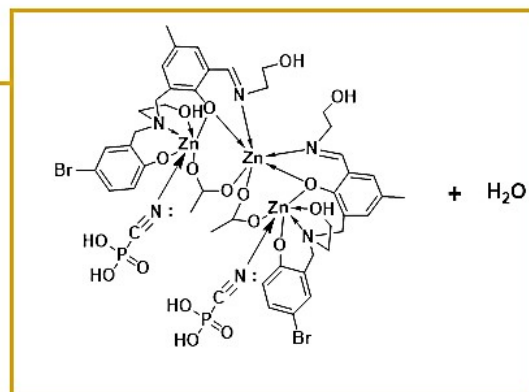
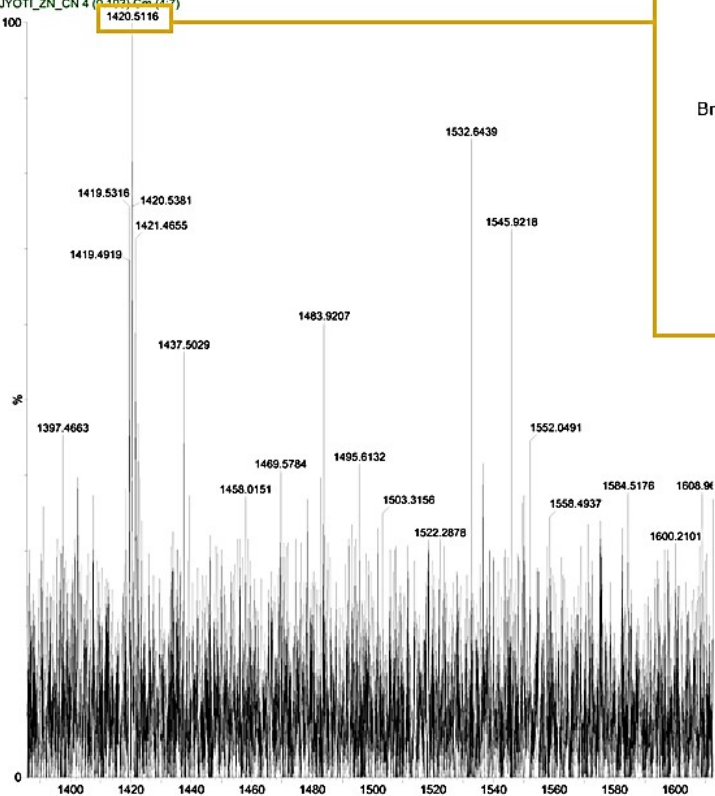


Figure S30 MS (m/z) showing the presence of hydrolyzed product formed after the addition of DCNP to trinuclear Zinc(II) cluster

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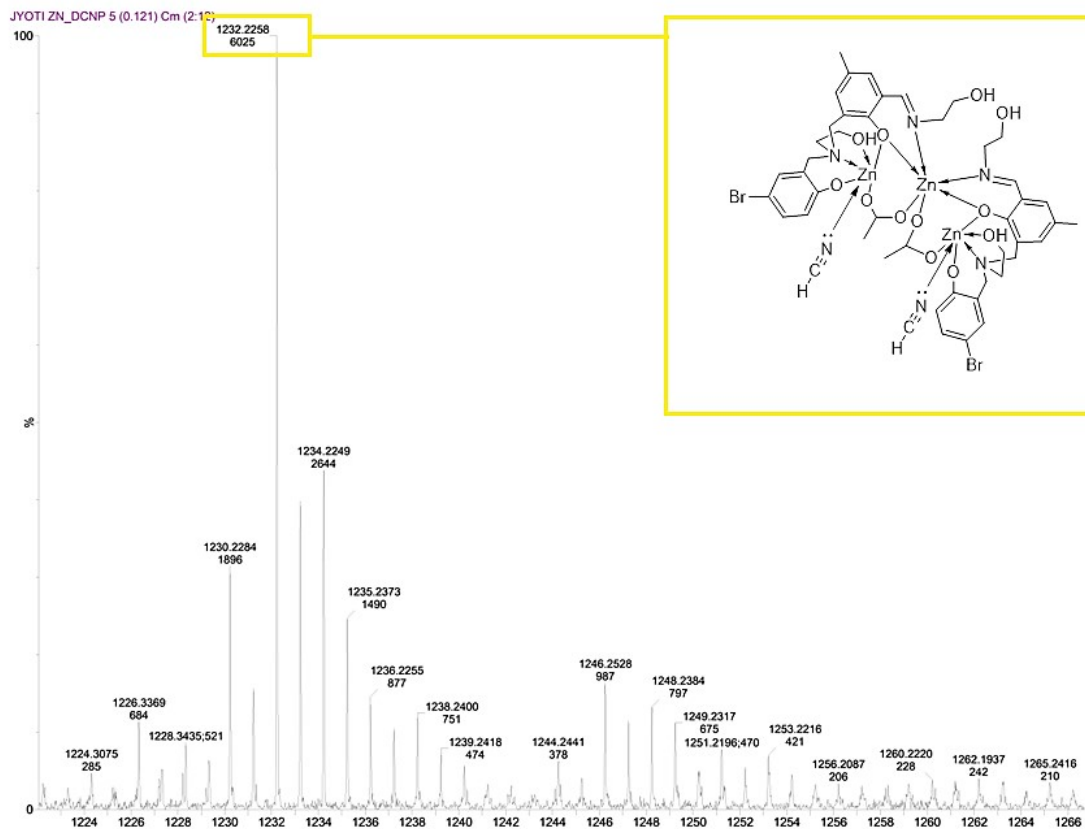


Figure S31 MS (m/z) of hydrolyzed product with HCN coordinated to trinuclear Zinc(II) cluster

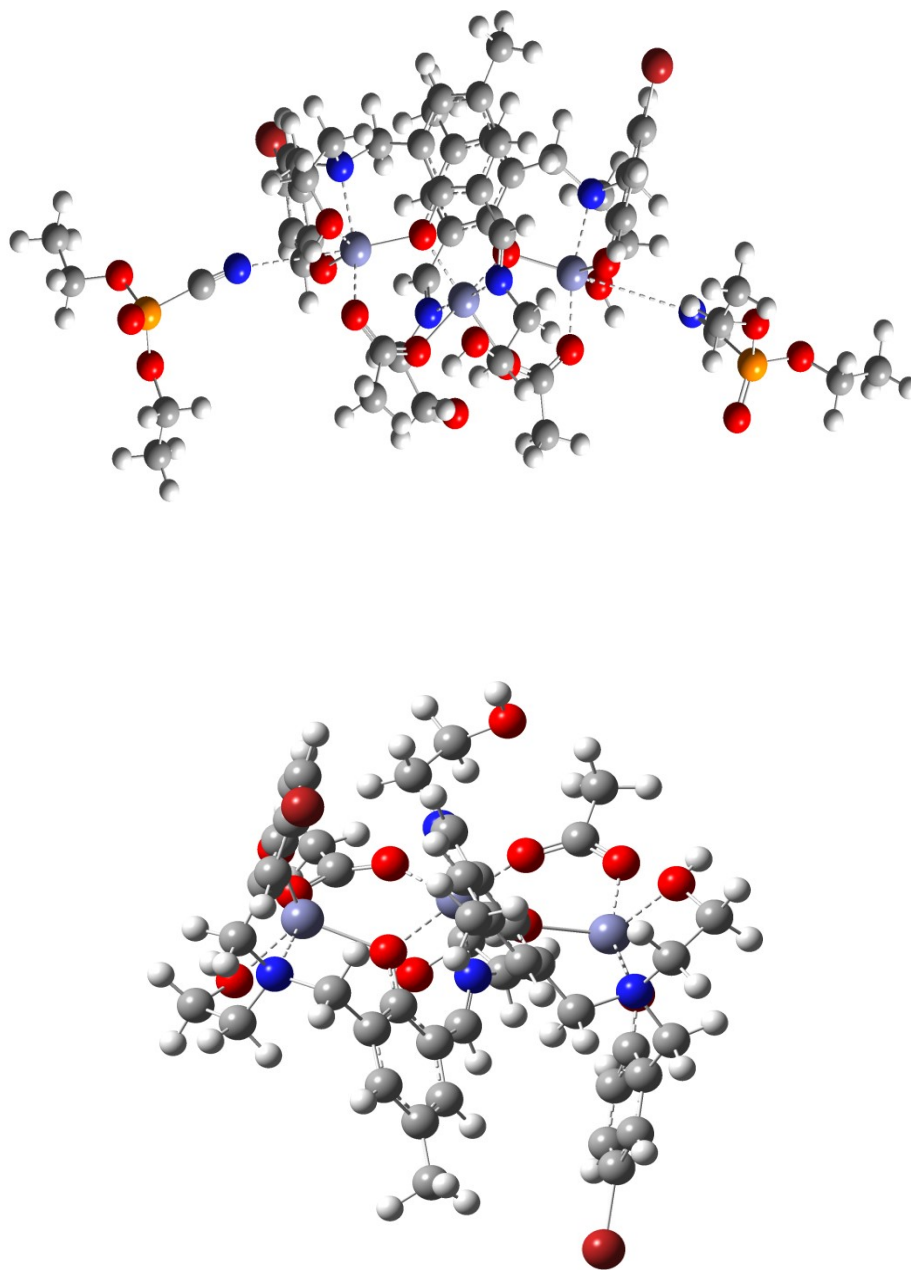


Figure S32 Optimized structures of trinuclear Zinc(II) cluster and its conjugate with DCNP using B3LYP/ LanL2DZ on Zn, Br, P and 6-31+G (d,p) on C, H, N, O.

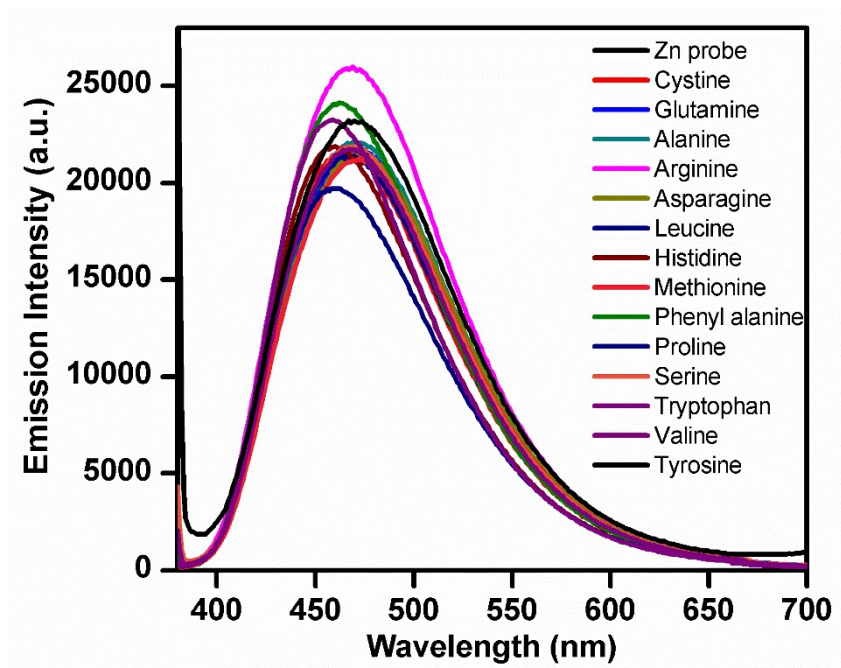


Figure S33 Comparison of emission intensity of the trinuclear Zinc(II) cluster in the presence of various Bio-relevant amino acids.

Table S1 Crystallographic data and structural parameters for trinuclear Zinc(II) cluster.

PARAMETERS	VALUE	PARAMETERS	VALUE
Empirical formula	C ₄₇ H ₆₀ Br ₂ N ₅ O ₁₃ Zn ₃	F(000)	1282.0
Formula weight	1257.93	Crystal size/mm ³	0.24 × 0.11 × 0.08
Temperature/K	285	Radiation	Mo Kα (λ = 0.71073)
Crystal system	Triclinic	2θ range for data collection/°	6.22 to 50.106
Space group	P-1	Index ranges	-12 ≤ h ≤ 12, -18 ≤ k ≤ 18, -20 ≤ l ≤ 20
a/Å	10.8217(6)	Reflections collected	42385
b/Å	15.4938(4)	Independent reflections	9976 [R _{int} = 0.0938, R _{sigma} = 0.1089]
c/Å	17.2737(5)	Data/restraints/parameters	9976/7/646
α/°	84.807(2)	Goodness-of-fit on F ²	0.990
β/°	83.062(4)	Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0581, wR ₂ = 0.1277
γ/°	80.267(3)	Final R indexes [all data]	R ₁ = 0.1155, wR ₂ = 0.1464
Volume/Å ³	2826.40(19)	Largest diff. peak/hole/ e Å ⁻³	0.67/-0.57
Z	2	ρ _{calc} g/cm ³	1.478
μ/mm ⁻¹	2.736		

Table S2 Bonding parameters for trinuclear Zinc(II) cluster.

Bond angles (°)					
O8 Zn3 O10	121.13(15)	O2 Zn1 O3	123.99(15)	O3 Zn2 O8	90.21(13)
O8 Zn3 N3	90.41(16)	O2 Zn1 O1	110.79(15)	O12 Zn2 O8	177.49(14)
O10 Zn3 N3	78.90(15)	O2 Zn1 O4	95.34(16)	O12 Zn2 O3	92.29(14)
O9 Zn3 O8	129.71(14)	O2 Zn1 N1	92.90(17)	O12 Zn2 O6	90.60(15)
O9 Zn3 O10	108.70(14)	O3 Zn1 O1	124.55(15)	O6 Zn2 O8	86.90(15)
O9 Zn3 O11	92.37(16)	O3 Zn1 O4	97.56(16)	O6 Zn2 O3	176.71(16)
O9 Zn3 N3	92.86(16)	O3 Zn1 N1	90.29(15)	N4 Zn2 O8	87.44(18)
O11 Zn3 O8	98.55(15)	O1 Zn1 N1	78.36(15)	N4 Zn2 O3	92.19(17)
O11 Zn3 O10	84.20(15)	O4 Zn1 O1	84.56(15)	N4 Zn2 O12	92.35(19)
O11 Zn3 N3	163.10(15)	O4 Zn1 N1	162.77(16)	N4 Zn2 O6	86.12(18)
Bond length (Å)					
Zn3-O8	2.025(4)	Zn1-O4	2.010(4)	Zn3-O10	2.111(3)
Zn1-N1	2.169(4)	Zn3-O9	1.973(4)	Zn2-O8	2.154(3)
Zn3-O11	2.005(4)	Zn2-O3	2.132(4)	Zn3-N3	2.163(4)
Zn2-O12	2.101(4)	Zn3-O2	1.968(4)	Zn2-O6	2.125(4)
Zn1-O3	2.008(4)	Zn2-N4	2.098(5)	Zn1-O1	2.126(3)
Zn2-N2	2.072(5)	Zn1-O8	2.025(4)	Zn2-O4	2.010(4)

Table S3. Readings of the emission measurements of trinuclear Zinc(II) cluster in the absence of analyte.

Blank Readings	Fluorescence Intensity
1	19689
2	19610
3	19440
4	19505
5	19660
6	19490
7	19505
8	19450
9	19550
10	19639
Standard Deviation (σ)	89.78

Table S4. Different compounds and corresponding methods for DCNP detection

S. No	Compound	Technique	Selectivity	Degradation	LOD	Reference
1	Hemicyanine-based	Fluorescence, Turn on	Yes	No	4.5 nM	[18]
2	Hydrazone-based Schiff base	Fluorescence, Turn off	No	Yes	158.2 nM	[23]
3	Imidazopyridine-based probe	Fluorescence, Turn off	No	No	3.6 μ M	[46]
4	Imidazo[1,2-a]pyridine	Fluorescence, Turn off	Yes	No	0.66 μ M and 0.54 μ M	[47]
5	Trinuclear Zinc cluster	Fluorescence, Turn off	Yes	Yes	186 nM	This work

Table S5 Calculated coordinates of trinuclear Zinc(II) cluster using B3LYP/ LanL2DZ on Zn, Br and 6-31+G (d,p) on C, H, N, O.

0,1

	X	Y	Z
Zn	-2.439830511	0.8973178653	-2.3400920514
Zn	2.435726774 4	0.874148798	2.3596215796
Zn	0.0003497551	1.9618300153	-0.0008607522
Br	-6.9546803136	-3.1638277802	1.9478923043
Br	6.9270240879	-3.1800932451	-1.9568076796
O	-0.7116574219	0.3947834874	-1.3660180058

O	4.21054 58746	1.061041849	1.4978994194
O	0.7102481943	0.4034260708	1.3746462768
O	-2.2251591076	0.6600098564	-4.5519133806
H	-2.4670064311	1.4969820 163	-4.9731594651
O	-4.2092207911	1.0849959861	-1.4743470679
O	-2.0881346566	2.810512339	-2.9553896396
O	2.2489086772	0.6336968143	4.5705125678
H	2.507166413	1.4577185705	5.0063856337
O	2.1165298063	2.799062848 2	2.9738515193
O	0.9461600767	3.5136479632	1.1864831754
N	-2.860873207 9	-1.3416032184	-2.7583121058
N	2.835457219	-1.3658409632	2.7587213742
O	-0.8801370155	3.512448183	-1.1910916386
N	1.8288266112	1.8396783493	-1.2290203149
N	-1.8164370766	1.8727213877	1.2269035666
O	1.950186635 8	4.0932992931	-3.2666140451
H	2.7682922931	3.9067013811	-3.7451577003
C	0.0431475205	-0.6312623032	-1.7497900903
C	2.5097852312	-1.67364809 5	4.169252688
H	2.9981863934	-2.6048809986	4.500091241
H	1.4298715993	-1.8163074848	4.246654063
C	-2.5381172241	-1.6425093811	-4.170856182
H	-3.0432977211	-2.5612860969	-4.5111931041
H	-1.4608831447	-1.80442686 83	-4.2483657134
C	-4.8297753599	0.1600561889	-0.7700914009
C	-0.53666 63745	-1.9108749118	-1.9871440022
C	-0.0593365678	-0.6149168783	1.7579 846405
C	-4.3097981711	-1.6068314771	-2.5144373779
H	-4.5063835934	-2. 6780730587	-2.6875051243
H	-4.8623565627	-1.0482963313	-3.2786442027
C	-1.6972949371	-2.8314707472	2.5718856665
C	-2.2353329476	-1.563576792 6	2.3798519701
H	-3.3011123572	-1.4102003752	2.534791453
C	1.9834489077	-2.1315885587	1.7992286181
H	2.2938500889	-1.8237227444	0.7967334473
H	2.2005902141	-3.2078819291	1.893000179
C	0.503967077	-1.9020365131	1.9883789858
C	4.8229174278	-1.2395192999	1.1649480858
C	-1.4582983017	-0.457489318	1.9723268735
C	4.8257494761	0.1366944044	0.7885439291
C	1.4455674185	-0.493004635	-1.9596539596
C	-2.0196037141	-2.1228510972	-1.802968589
H	-2.2489413962	-3.1961490803	-1.90286004
H	-2.327663592	-1.8176813769	-0.7989003889
C	4.2807282691	-1.6453323743	2.5116789537
H	4.4646905567	-2.720776735	2.6716677769
H	4.8402685233	-1.1030942143	3.2824987786
C	-6.113946289	-1.7909164295	0.8168346999
C	-0.3135950114	-2.9656357814	2.3739532534
H	0.147461433	-3.9412486499	2.5253465711
C	-5.4723342721	-2.1704028455	-0.357154645
H	-5.4698844624	-3.213086502 9	-0.6622627687
C	2.2097114057	-1.6092293075	-2.3667770572

H	3.2782785732	-1.4704735047	-2.5171531636
C	-4.8448309353	-1.2113507712	-1.16223 2852
C	0.2681819172	-2.9833429621	-2.372468982
H	-0.2055204778	-3.9519 633852	-2.5294575471
C	-5.5402054043	0.5073846552	0.4067571238
H	-5.58 47281912	1.5568678828	0.6803008555
C	6.1752455778	-0.4674049626	-1.176 2871693
H	6.7171955729	-0.167999177	-2.0678483136
C	-2.9042572774	-0.4810793266	-5.0911461876
H	-2.5514835073	-0.6919975966	-6.1078202853
H	-3.9853319581	-0.2998452374	-5.1247039122
C	1.6552585885	-2.8683538991	-2.5640708952
C	1.5212415176	3.696509702	2.2911043753
C	2.8998628904	-0.5288658839	5.100191349
H	2.5392668144	-0.7404890161	6.113845236
H	3.984574214	-0.3721844871	5.1381723459
C	-6.1722374313	-0.4509881674	1.1966312426
H	-6.7023848803	-0.1554994215	2.0964787933
C	5.4433689593	- 2.1960968344	0.3516988236
H	5.4264372492	-3.2421952073	0.6442966002
C	5.5495988542	0.4889647724	-0.3787837868
H	5.6109883593	1.5415859536	-0 .6370724539
C	-1.4391334072	3.6970796395	-2.3074099642
C	6.0968047949	-1.8110391827	-0.814114409
C	-2.1838481642	0.8019007545	1.837998189
H	-3.1741868951	0.7884808328	2.3071387742
C	2.1853749923	0.7563149084	-1 .8257985099
H	3.1820205573	0.7227644204	-2.282883552
C	-2.7717754602	2.9872396243	1.2312622446
H	-3.6855270097	2.7032994762	1.770038172
H	- 3.0423671056	3.2048189045	0.1942113435
C	2.240761664	4.2219353277	-1.8719412445
H	1.3000270876	4.4968549401	-1.3945050137
H	2.9694518957	5.0288527287	-1.7018226239
C	2.7919893186	2.9431007786	-1.242710971
H	3.7093580891	2.6390822871	-1.7712222062
H	3.0703447862	3.1646192101	-0.20 75223228
C	-2.54862987	-4.0056516543	2.9997689324
H	-2.3344367574	-4.3 022960058	4.0345668592
H	-2.3664391255	-4.8834837242	2.3687782434
H	-3 .6140115317	-3.7672533396	2.9377781974
C	2.4912771465	-4.0547457126	-2.9882232701
H	3.5585464404	-3.8180934294	-2.9610739618
H	2.2472324164	-4.3751930768	-4.009091212
H	2.3251903181	-4.9172495275	-2.3319172613
O	-2.0463234488	4.0270514659	3.263913545
H	-1.51667686	4.7418092918	3. 6363598284
C	-2.2060274694	4.2521267978	1.8574605951
H	-1.2518097864	4.5049096084	1.3856590371
H	-2.9223457267	5.0686277716	1.6800643572
C	- 1.3237016406	5.0683356466	-2.9459610137
H	-2.1317376159	5.2377074134	- 3.6602296591
H	-0.3645230673	5.1106418355	-3.4751248462

H	-1.3212116861	5.8470054113	-2.1794616948
C	1.558016016	5.1045925283	2.8668912206
H	0.895637302	5.7745881964	2.3158732109
H	2.582539934	5.4873590854	2.8013764089
H	1.2914954161	5.0840993749	3.9279383855

Table S6 Calculated coordinates of trinuclear Zinc(II) cluster-DCNP using B3LYP/ LanL2DZ on Zn, Br, P and 6-31+G (d,p) on C, H, N, O.

0 1

	X	Y	Z
Zn	-3.2483198	0.03569371	1.37242644
Zn	3.13752053	-0.4568543	-1.0323567
Zn	-0.0750242	-1.2538923	0.35697883
Br	-6.2470582	3.23476973	-4.7391408
Br	6.01637844	4.83509359	3.50070939
O	-1.2601847	0.45112573	1.03690225
O	4.17948534	-0.2363942	0.63737722
O	1.13999718	0.03567963	-0.9235755
O	-3.9101693	0.62687778	3.45517466
H	-4.3755386	-0.1355267	3.82777616
O	-4.3691419	-0.4092202	-0.2116929
O	-3.1823389	-1.7576589	2.34005997
O	3.85673983	-0.6085835	-3.2170403
H	4.33649116	-1.4468642	-3.2817156
O	3.0780769	-2.4862808	-1.2524488
O	1.25900888	-2.9512917	-0.0041301
N	-3.7835441	2.24919162	1.21563209
N	3.65954026	1.69092826	-1.7167663
O	-1.3679465	-2.6678367	1.3599365
N	1.09915631	-0.7942273	2.17074311
N	-1.2306856	-1.5409581	-1.4939592
O	0.38589519	-2.6565057	4.47095958
H	0.93083015	-2.2595303	5.16296477
C	-0.7092198	1.59156486	1.4435615
C	3.87645495	1.7490025	-3.1794569
H	4.43379335	2.65596755	-3.4671993
H	2.90128817	1.78908062	-3.6674139
C	-3.9628154	2.81610451	2.57260576
H	-4.5244969	3.76382199	2.534031
H	-2.9756213	3.02999948	2.98560215

C	-4.8239547	0.39177368	-1.1489506
C	-1.3387934	2.84427844	1.18622561
C	0.5862791	0.93640306	-1.7317744
C	-5.066697	2.35634035	0.46362687
H	-5.3536369	3.41953711	0.41405176
H	-5.8232721	1.84333948	1.06864704
C	-0.616397	2.89888691	-3.4528679
C	-1.1895903	1.64485734	-3.2726609
H	-2.1177262	1.40499361	-3.7875427
C	2.51215021	2.54503789	-1.2774105
H	2.42789912	2.4199847	-0.1944674
H	2.74999105	3.60445292	-1.464799
C	1.20333948	2.20223876	-1.9495103
C	4.90087044	2.06198145	0.49258497
C	-0.6268725	0.66469143	-2.4275605
C	4.63224406	0.85476018	1.20834747
C	0.51279923	1.60594159	2.17623617
C	-2.6650089	2.90409353	0.46669056
H	-2.9208511	3.9566313	0.26413318
H	-2.5962342	2.39655983	-0.499116
C	4.91579473	2.08449697	-1.0172554
H	5.19651199	3.09657596	-1.353062
H	5.69501735	1.39844069	-1.3692752
C	-5.7011463	2.05550202	-3.2611596
C	0.59147054	3.14350081	-2.7791429
H	1.08008067	4.10865156	-2.9098922
C	-5.5044778	2.59097278	-1.9931049
H	-5.6889368	3.64707792	-1.8176838
C	1.07747404	2.83429536	2.5826809
H	2.01377368	2.80921785	3.1367461
C	-5.088174	1.77763346	-0.9302039
C	-0.72738	4.02971699	1.59625851
H	-1.2262542	4.97139061	1.36885694
C	-5.0897603	-0.1193468	-2.4468439
H	-4.9417658	-1.1826945	-2.6090336
C	5.29643364	2.01054009	3.2808273
H	5.46841884	1.98440768	4.35228375
C	-4.6705959	1.83981869	3.50861031
H	-4.6619348	2.24449116	4.5281979
H	-5.7053442	1.64453343	3.21238555
C	0.49391155	4.06121608	2.28987334

C	2.23208819	-3.2824619	-0.7290925
C	4.61120314	0.51410809	-3.6897867
H	4.62674915	0.5273421	-4.7866155
H	5.64047072	0.45136684	-3.3206544
C	-5.5164811	0.69425296	-3.4940897
H	-5.6967417	0.27260663	-4.4779532
C	5.30347974	3.21352704	1.1826887
H	5.49213291	4.12937737	0.62948707
C	4.88153584	0.86469635	2.60649956
H	4.73810171	-0.065407	3.14818046
C	-2.3284088	-2.6912503	2.17766335
C	5.48445519	3.18852201	2.56088657
C	-1.343465	-0.6048605	-2.368454
H	-2.0771274	-0.7319497	-3.1728147
C	1.22916252	0.41027526	2.60206263
H	1.98244838	0.60515096	3.37583595
C	-2.1046667	-2.7057901	-1.6645306
H	-2.7117284	-2.5986315	-2.5742137
H	-2.7819834	-2.7418018	-0.8069861
C	1.21444112	-2.9937799	3.35473211
H	0.54620016	-3.4142299	2.60299857
H	1.95000092	-3.7617763	3.64061298
C	1.97287673	-1.8034634	2.77051522
H	2.60112761	-1.3454393	3.55211189
H	2.64640402	-2.1727885	1.9908627
C	-1.241473	3.94233256	-4.3516009
H	-0.6498875	4.0965344	-5.2632106
H	-1.3153849	4.91328047	-3.8477877
H	-2.2497919	3.64959864	-4.6577157
C	1.11966806	5.36902411	2.7199114
H	2.11819193	5.21190729	3.13742397
H	0.51530562	5.87395959	3.48430553
H	1.21810236	6.06310374	1.87687104
O	-0.6348323	-4.0635199	-2.9854162
H	0.0555941	-4.7343963	-2.9304469
C	-1.338854	-4.016889	-1.7371247
H	-0.651351	-4.0887581	-0.8895703
H	-2.0647715	-4.8428063	-1.6804019
C	-2.4785382	-3.9152734	3.062595
H	-3.5027065	-4.0158171	3.42724827
H	-1.8067134	-3.7882578	3.92003612

H	-2.1709781	-4.8156373	2.52531317
C	2.47583531	-4.7657166	-0.9802577
H	1.62532602	-5.3672598	-0.653877
H	3.36245506	-5.0800142	-0.4179304
H	2.69006673	-4.938142	-2.0392716
P	-8.6638136	-2.5633079	1.45368682
O	-10.094489	-1.9948719	2.03207469
O	-8.7278395	-2.1262454	-0.1366974
O	-8.2487327	-3.9869624	1.77146447
C	-11.310515	-2.7658778	1.77763354
H	-11.498965	-2.7650012	0.69982113
H	-11.151038	-3.7942491	2.11440329
C	-7.6680799	-2.5753037	-1.0438337
H	-7.5129073	-3.6473917	-0.8981468
H	-6.7496859	-2.0366599	-0.7878405
C	-8.1230617	-2.249196	-2.4518027
H	-7.3500328	-2.5560001	-3.1634047
H	-9.0484934	-2.7780029	-2.6959874
H	-8.2895915	-1.1751527	-2.5647257
C	-12.433421	-2.0922566	2.54067966
H	-13.368247	-2.6362368	2.37158209
H	-12.224257	-2.0868384	3.61345745
H	-12.566436	-1.0610018	2.20403886
C	-7.567612	-1.288636	2.18710871
N	-6.7746471	-0.5227639	2.53602827
P	9.31055238	-2.5928506	-1.5820176
O	10.1697729	-1.3109167	-1.0206051
O	9.21099578	-3.5649692	-0.2477917
O	9.70652212	-3.267469	-2.8819959
C	11.6211456	-1.4329558	-0.8752608
H	11.8259349	-2.1837433	-0.1063669
H	12.0411291	-1.7677394	-1.8280731
C	8.71361584	-4.9312314	-0.396851
H	9.22940702	-5.4061103	-1.235299
H	7.64128693	-4.8840961	-0.6183629
C	8.9752053	-5.6456641	0.91406808
H	8.60229822	-6.6727766	0.85055116
H	10.0459969	-5.6790757	1.13210482
H	8.46556935	-5.1420335	1.73934108
C	12.1440162	-0.0677109	-0.4769018
H	13.2300943	-0.1160701	-0.3495237

H	11.9177296	0.67420302	-1.2468827
H	11.6978656	0.25877747	0.46576365
C	7.66625346	-1.7847589	-1.6573684
N	6.59857068	-1.3409073	-1.7097497