

## Electronic Supporting Information

### **Strategically synthesized Arseno-discriminatory terta-phenoxido hetero-trinuclear complex envisioned for recognition of *i*As and *o*As from *Oryza sp.* and aquatic crustacean**

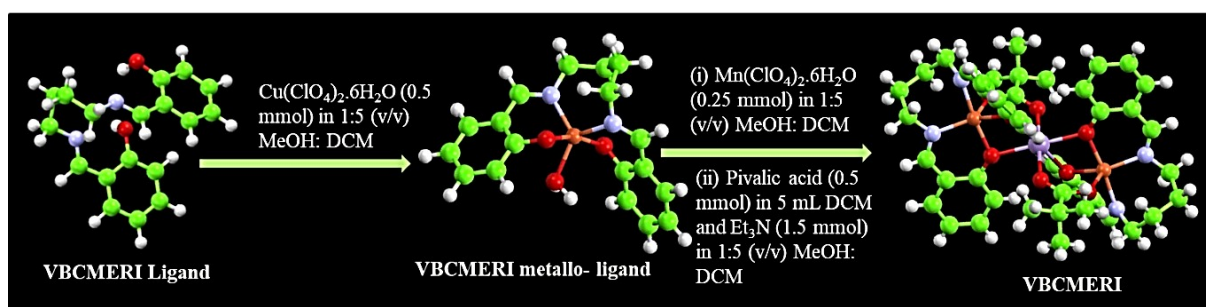
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**Fig.S1.** Synthetic scheme of VBCMERICl

**Table S1:** Crystallographic data of VBCMERICl

<b>Crystal Data</b>	
Formula	C <sub>46</sub> H <sub>54</sub> Cu <sub>2</sub> Mn N <sub>4</sub> O <sub>8</sub>
Formula Weight	972.97
Crystal System	triclinic
Space group	P-1(No. 2)
a, b, c [Angstrom]	9.3404(10) 10.8427(11) 10.9733(12)
alpha, beta, gamma [deg]	99.826(7) 105.966(7) 90.367(7)
V [Ang**3]	1051.1(2)
Z	1
D(calc) [g/cm**3]	1.537
Mu(MoKa) [ /mm ]	1.359
F(000)	505
Crystal Size [mm]	0.18 x 0.28 x 0.36
<b>Data Collection</b>	
Temperature (K)	296
Radiation [Angstrom]	MoKa 0.71073
Theta Min-Max [Deg]	3.0, 28.3
Dataset	-12: 12 ; -14: 14 ; -14: 14
Tot., Uniq. Data, R(int)	33387, 5122, 0.148
Observed Data [I > 2.0 sigma(I)]	2994

**Table S2:** Selected bond distances (angstrom) of VBCMERICl

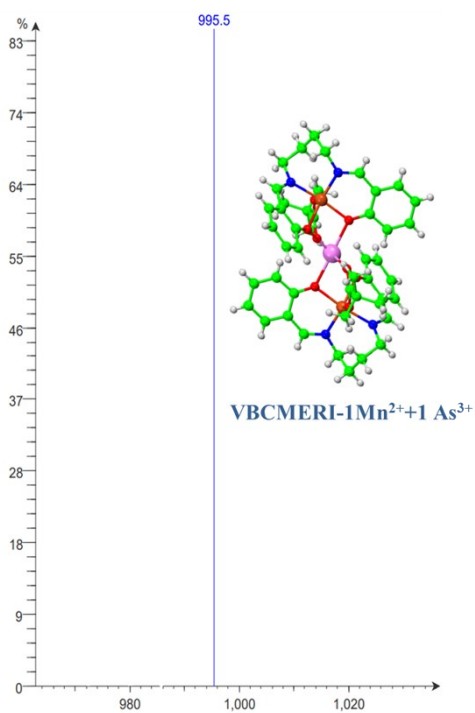
Cu1	-O1	1.925(3)	C10	-C11	1.496(9)
Cu1	-O2	2.017(4)	C12	-C13	1.423(8)
Cu1	-O4	2.070(4)	C13	-C14	1.389(9)
Cu1	-N1	1.968(4)	C13	-C18	1.413(8)
Cu1	-N2	1.984(5)	C14	-C15	1.353(10)
Mn1	-O1	2.228(4)	C15	-C16	1.390(11)
Mn1	-O2	2.193(3)	C16	-C17	1.362(10)
Mn1	-O3	2.209(4)	C17	-C18	1.389(8)
Mn1	-O1_a	2.228(4)	C19	-C20	1.523(8)
Mn1	-O2_a	2.193(3)	C20	-C22	1.40(2)
Mn1	-O3_a	2.209(4)	C20	-C23	1.419(17)
O1	-C1	1.309(7)	C20	-C24	1.39(2)
O2	-C18	1.314(6)	C2	-H2	0.9300
O3	-C19	1.244(7)	C3	-H3	0.9300
O4	-C19	1.238(8)	C4	-H4	0.9300
N1	-C11	1.449(8)	C5	-H5	0.9300
N1	-C12	1.277(7)	C7	-H7	0.9300
N2	-C7	1.269(8)	C8	-H8A	0.9700
N2	-C8	1.457(8)	C8	-H8B	0.9700
C1	-C2	1.383(8)	C9	-H9A	0.9700
C1	-C6	1.416(8)	C9	-H9B	0.9700
C2	-C3	1.379(9)	C10	-H10A	0.9700
C3	-C4	1.372(10)	C10	-H10B	0.9700
C4	-C5	1.360(9)	C11	-H11A	0.9700
C5	-C6	1.391(9)	C11	-H11B	0.9700
C6	-C7	1.422(9)	C12	-H12	0.9300

**Table S3:** Selected bond angles (degrees) of VBCMERI

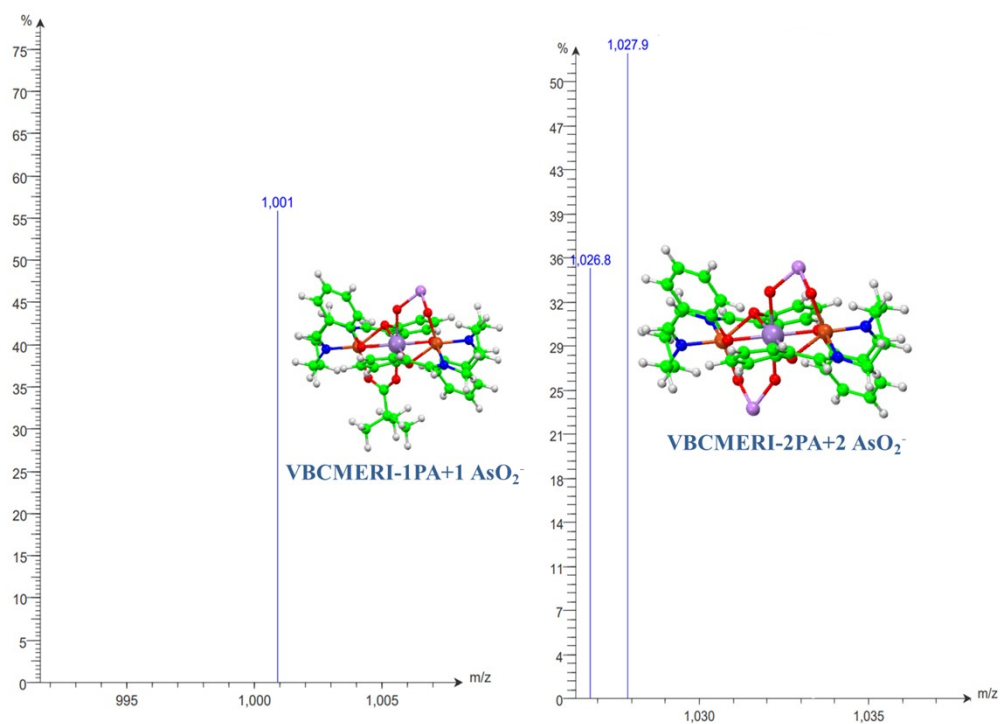
C12	-C13	-C18	122.0(5)	N2	-C8	-H8A	109.00
C14	-C13	-C18	119.4(5)	N2	-C8	-H8B	109.00
C13	-C14	-C15	121.6(6)	C9	-C8	-H8A	109.00
C14	-C15	-C16	118.8(7)	C9	-C8	-H8B	109.00
C15	-C16	-C17	121.2(7)	H8A	-C8	-H8B	108.00
C16	-C17	-C18	120.7(6)	C8	-C9	-H9A	108.00
O2	-C18	-C13	121.8(5)	C8	-C9	-H9B	108.00
O2	-C18	-C17	120.2(5)	C10	-C9	-H9A	108.00
C13	-C18	-C17	118.1(5)	C10	-C9	-H9B	108.00
O3	-C19	-O4	125.4(5)	H9A	-C9	-H9B	107.00
O3	-C19	-C20	120.3(6)	C9	-C10	-H10A	108.00
O4	-C19	-C20	114.3(5)	C9	-C10	-H10B	108.00
C19	-C20	-C22	114.1(8)	C11	-C10	-H10A	108.00
C19	-C20	-C23	110.3(8)	C11	-C10	-H10B	108.00
C19	-C20	-C24	109.3(9)	H10A	-C10	-H10B	107.00
C22	-C20	-C23	114.7(16)	N1	-C11	-H11A	109.00
C22	-C20	-C24	105.2(15)	N1	-C11	-H11B	109.00
C23	-C20	-C24	102.4(19)	C10	-C11	-H11A	109.00
C1	-C2	-H2	119.00	C10	-C11	-H11B	109.00
C3	-C2	-H2	119.00	H11A	-C11	-H11B	108.00
C2	-C3	-H3	120.00	N1	-C12	-H12	117.00
C4	-C3	-H3	120.00	C13	-C12	-H12	117.00
C3	-C4	-H4	120.00	C13	-C14	-H14	119.00
C5	-C4	-H4	120.00	C15	-C14	-H14	119.00
C4	-C5	-H5	119.00	C14	-C15	-H15	121.00
C6	-C5	-H5	119.00	C16	-C15	-H15	121.00

**Table S4:** Hydrogen bonding in VBCMERI

C8	--H8A	..N1	0.9700	2.5200	2.900(8)	103.00
C10	--H10B	..O4	0.9700	2.4200	3.145(8)	132.00
C17	--H17	..O3	0.9300	2.5400	3.255(8)	133.00
C22	--H22C	..O3	0.9600	2.2800	2.738(16)	108.00
C23	--H23B	..O4	0.9600	2.3100	2.656(19)	100.00



**Fig.S2.** ESI-MS spectra of VBCMERI with  $\text{As}^{3+}$



**Fig.S3.** ESI-MS spectra of VBCMERI with  $\text{AsO}_2^-$

**Table S5: CARTESIAN COORDINATES of VBCMERI\_T (ANGSTROM)**

Mn	2.926609	5.004230	4.940842
Cu	1.138995	6.670271	6.610474
O	2.766658	7.101748	5.429377
O	3.439106	4.599709	6.998305

O	0.795292	5.035682	5.380290
O	1.993799	5.917732	8.215822
N	1.008729	8.679610	6.841376
N	-0.865796	6.580274	6.915331
C	0.811314	9.230750	8.183729
C	1.077188	9.460868	5.807321
C	-1.705945	7.777223	6.939375
C	-0.848994	3.180521	8.193946
C	2.381561	7.904027	4.319934
C	0.379060	3.978254	6.244024
C	-0.249336	8.454182	8.966548
C	-0.509069	4.225061	7.317786
C	1.468532	8.970198	4.476453
C	3.549124	4.496743	9.455201
C	-1.641113	8.476616	8.308106
C	0.630697	2.641139	5.904195
C	-1.313441	5.456465	7.378035
C	0.291435	1.603380	6.775192
C	2.958316	5.023688	8.157867
C	1.132403	9.765218	3.366672
C	-0.404737	1.881700	7.948945
C	3.118477	7.834151	3.126293
C	1.758853	9.565774	2.136587
C	2.779168	8.624340	2.026426
C	2.419393	4.235882	10.472214
C	4.308536	3.175571	9.211619
C	4.520013	5.546926	10.021141
O	5.038326	5.164861	4.511426
O	3.135637	2.902501	4.505551
O	2.390611	5.270780	2.860566
H	1.776848	9.170846	8.736044
H	0.511079	10.305888	8.147863
H	0.896205	10.531354	5.919322
H	-1.394881	8.470129	6.129455
H	-2.766675	7.513691	6.711540
H	-1.509038	3.361831	9.037909
H	-0.339223	8.919826	9.975494
H	0.086717	7.407464	9.137160
H	-2.352196	7.963848	8.997052
H	-1.988939	9.530176	8.198975

H	0.991154	2.383193	4.923593
H	-2.327181	5.394830	7.778380
H	0.527638	0.576091	6.515636
H	0.422253	10.581497	3.468753
H	-0.682817	1.075495	8.620511
H	3.959203	7.158986	3.039998
H	1.500773	10.189829	1.286675
H	3.323276	8.519643	1.092914
H	2.832165	3.822905	11.421830
H	1.875868	5.178155	10.716528
H	1.685581	3.504176	10.060433
H	5.163372	3.331572	8.513185
H	4.716208	2.773231	10.168024
H	3.627993	2.409783	8.771096
H	5.343635	5.748670	9.297171
H	3.988542	6.506268	10.222131
H	4.971475	5.190600	10.976170
H	5.304696	6.123955	4.789321
H	5.132880	5.145085	3.483041
H	3.659827	2.513686	5.307216
H	3.798398	2.844795	3.714957
H	3.055445	4.696171	2.317328
H	1.484689	4.785024	2.754507

**Table S6: CARTESIAN COORDINATES of VBCMERI\_T+ Arsenobetaine (ANGSTROM)**

Mn	2.768395	5.131957	4.332668
Cu	1.285501	6.789079	6.294413
O	2.596046	7.233484	4.771888
O	3.849424	4.956088	6.207576
O	0.886534	5.038590	5.331979
O	2.530965	6.164235	7.699032
N	1.159292	8.793317	6.538288
N	-0.732705	6.650776	6.751236
C	1.096923	9.308957	7.904742
C	1.054227	9.587282	5.513894
C	-1.538281	7.868976	6.846809
C	-0.825194	3.281527	8.112558
C	1.954342	8.000997	3.767874
C	0.691498	4.111183	6.396206
C	0.101619	8.511110	8.750105
C	-0.441965	4.286256	7.209655

C	1.145937	9.102537	4.122938
As	3.927902	4.011252	9.909452
C	-1.342016	8.556195	8.210768
C	1.493454	2.974358	6.592853
C	-1.246122	5.516004	7.136397
C	1.109507	1.981221	7.499380
C	3.604923	5.442507	7.422428
C	0.582628	9.902014	3.112970
C	-0.056129	2.127069	8.247412
C	2.363880	7.875975	2.430566
C	0.880433	9.663193	1.771009
C	1.797201	8.670476	1.432013
C	2.063052	4.438620	10.366178
C	4.118206	2.144490	9.325014
C	5.028679	4.254822	11.521029
O	4.644144	5.392843	3.304358
O	2.917126	3.019826	3.900337
O	1.663575	5.254655	2.481179
C	4.612710	5.215591	8.508978
H	2.107905	9.219659	8.363747
H	0.809446	10.387779	7.928345
H	0.877998	10.653053	5.668566
H	-1.285252	8.555899	6.014399
H	-2.622657	7.642060	6.706364
H	-1.712812	3.400396	8.727730
H	0.099629	8.944855	9.777072
H	0.448032	7.457802	8.856392
H	-1.997679	8.045647	8.954216
H	-1.684444	9.614776	8.141109
H	2.427710	2.844210	6.088089
H	-2.274801	5.477021	7.499777
H	1.719817	1.092487	7.623824
H	-0.054007	10.744873	3.368381
H	-0.350747	1.355420	8.951693
H	3.139120	7.170314	2.157817
H	0.448666	10.291146	0.997898
H	2.090698	8.533503	0.395894
H	1.695583	3.723591	11.134779
H	2.009082	5.475892	10.764502
H	1.432497	4.363394	9.457461



H	5.176787	1.827147	9.451386
H	3.457774	1.491731	9.937642
H	3.846239	2.064283	8.251704
H	6.089403	4.017866	11.283919
H	4.951528	5.309996	11.865019
H	4.665741	3.574957	12.323281
H	5.117083	6.157911	3.813718
H	3.921738	2.797967	4.001285
H	2.223121	4.715284	1.799575
H	4.864306	6.193932	8.976687
H	5.546956	4.780188	8.087390

**Table S7: CARTESIAN COORDINATES of VBCMERI\_T+Arsenobetaine+As<sup>3+</sup> (ANGSTROM)**

As	2.974710	5.367775	4.693049
Cu	1.368060	6.991251	6.415360
O	2.664433	7.258596	4.890129
O	3.875772	5.258044	6.379668
O	1.125029	5.354555	5.251009
O	2.533379	6.426711	7.863146
N	1.225749	8.998496	6.479481
N	-0.558275	6.759185	6.939722
C	1.141116	9.657780	7.781159
C	1.126449	9.666602	5.373423
C	-1.422145	7.931784	7.076042
C	-0.432224	3.265589	7.957060
C	1.872293	7.813935	3.821035
C	0.814285	4.237344	6.093311
C	0.324161	8.822554	8.774376
C	-0.109900	4.380137	7.162377
C	1.116149	8.986750	4.067788
As	3.773229	4.040125	9.908665
C	-1.162010	8.675079	8.396981
C	1.178701	2.925204	5.716836
C	-0.941751	5.588933	7.342542
C	0.842062	1.826687	6.508289
C	3.601796	5.715360	7.597174
C	0.398388	9.599491	3.027008
C	0.070592	2.003350	7.651427
C	1.965070	7.364643	2.480109
C	0.437990	9.081291	1.736005
C	1.232058	7.974322	1.460451

C	2.006093	4.618402	10.552973
C	3.621415	2.333896	8.946680
C	4.964783	3.791942	11.453342
O	4.441061	6.119562	3.728898
O	3.806395	3.646954	4.667848
O	2.526310	4.368455	3.127203
C	4.546523	5.402658	8.714620
H	2.172475	9.787059	8.181613
H	0.677020	10.669963	7.696358
H	0.961279	10.744972	5.399663
H	-1.261797	8.612084	6.212571
H	-2.498073	7.637721	7.028753
H	-1.119033	3.365633	8.793373
H	0.374362	9.328919	9.766304
H	0.783113	7.821149	8.915292
H	-1.669742	8.116142	9.217355
H	-1.634462	9.683638	8.345332
H	1.710286	2.732631	4.795512
H	-1.925997	5.471716	7.799783
H	1.170473	0.831661	6.224545
H	-0.188723	10.494739	3.214678
H	-0.193441	1.148706	8.266336
H	2.625226	6.568398	2.182034
H	-0.120277	9.562486	0.938837
H	1.302914	7.600883	0.443337
H	1.581916	3.836725	11.220958
H	2.112745	5.572152	11.115417
H	1.325703	4.775261	9.689393
H	4.638931	1.938139	8.733983
H	3.058144	1.603728	9.568928
H	3.087436	2.503368	7.988934
H	5.966449	3.462582	11.098790
H	5.062576	4.754227	12.002908
H	4.537107	3.019376	12.130001
H	5.222544	6.173441	4.403250
H	4.577556	3.430860	4.011048
H	3.417842	4.091975	2.683010
H	4.746639	6.326968	9.301905
H	5.512115	5.022885	8.309975

**Table S8: CARTESIAN COORDINATES of VBCMERI\_T+As<sup>3+</sup> (ANGSTROM)**

1 as	5.12004724396150	9.12555464141398	9.51163185957555
2 cu	1.32580541706225	12.70723271080776	13.05185540050081
3 o	4.28428921926404	12.70559829379307	10.05727634034544
4 o	6.59986934587562	9.02948339203579	12.84400126449412
5 o	1.74100535465391	8.72181624536708	10.95751411786224
6 o	3.76064568712713	10.82986808306138	15.53986595969475
7 n	1.65221578613886	16.42011362573701	13.28152866120646
8 n	-2.30008075507583	11.89060823762010	12.66570474987530
9 c	0.37325564340308	17.65597402870070	15.41956185122451
10 c	2.34407883293816	17.84886914288456	11.40237349113677
11 c	-3.95226363162010	14.11490860706054	12.72137096235060
12 c	-3.41249099864280	5.19253565939268	13.98296031418817
13 c	4.53799283107615	14.63514564413891	8.37839607064498
14 c	0.55803465004146	6.80771749658799	12.17521506808109
15 c	-1.56823105476971	15.94401122757967	16.73466928599608
16 c	-2.01842922585164	7.24059983545476	12.94877220861964
17 c	3.65654229102867	17.12141433469827	9.08262386135174
18 c	7.68617113276515	9.09702589948429	17.22122316818745
19 c	-4.07011300968874	15.40224126065692	15.34435773458138
20 c	1.65191673611522	4.41837624729717	12.66796862421245
21 c	-3.33617976780095	9.66754152785939	12.83584992249682
22 c	0.23366185639194	2.46506668302882	13.76715254080896
23 c	5.78629207470083	9.74339276984122	15.09504345610146
24 c	4.01572371424892	19.14421532511426	7.34139584440775
25 c	-2.32475953113519	2.82134086372314	14.40427490570036
26 c	5.65301580307562	14.33668762496432	5.96055066387595
27 c	5.15305631201839	18.81972053156845	4.98450364640971
28 c	5.95989131568524	16.37942281970816	4.30361537222546
29 c	6.60737937198063	9.95607970188053	19.78443914155784
30 c	8.14187375617605	6.20726920597968	17.23621542173392
31 c	10.19838498317096	10.49590090220434	16.67157936176364
32 o	8.17391531864236	10.06015410998659	8.26905697387677
33 o	5.96214944548322	5.77049945820067	9.39062788812939
34 o	3.59868892581064	9.05370267493549	6.42486516112501
35 h	1.85852398718013	18.13873899453950	16.83344108789386
36 h	-0.51376927294763	19.47491029879355	14.81325577321912
37 h	1.86975426797543	19.89914604646831	11.49155346482743
38 h	-3.23262865447873	15.47617981347309	11.28987573685538
39 h	-5.91684483629258	13.59321966605241	12.15846191816280
40 h	-5.40388773136551	5.52873330831645	14.50571943164921

41 h	-2.05837149169199	16.85852990988201	18.56572631209127
42 h	-0.61251120044093	14.13303260319580	17.23214436758928
43 h	-5.24309894042986	14.19357360912282	16.60781064069591
44 h	-5.13525581790991	17.20176931004871	15.09327224805252
45 h	3.62326951939238	4.10326252725262	12.10115580750347
46 h	-5.43241740849382	9.54320199560646	13.02751907107873
47 h	1.14764370962004	0.62155835654157	14.10369512753323
48 h	3.34431319367816	21.03595300314422	7.90678058113278
49 h	-3.44713511259233	1.27446472344238	15.23020801784886
50 h	6.30113612894384	12.45896569491130	5.38546598574353
51 h	5.39878065709148	20.43377235817343	3.69261192173609
52 h	6.85405565456086	16.04647556612661	2.45000886238922
53 h	7.97704010823510	9.50193748361487	21.31327623802446
54 h	6.25066236245313	12.02495843553132	19.80948777452390
55 h	4.79487781976008	8.98687445720616	20.21648400316223
56 h	8.91867053743033	5.55329724585264	15.40021194635915
57 h	9.51011767658749	5.71295937474323	18.75488705396281
58 h	6.35646343302862	5.15898381290527	17.60425621566161
59 h	11.02683525635886	9.88076725328831	14.84387369265086
60 h	9.91049304523678	12.57799109376080	16.59774830577816
61 h	11.58493043760453	10.08634786928046	18.19903766271413
62 h	9.30893611932774	8.65301305053740	8.72894440737565
63 h	5.29595079166857	5.18937856495646	7.74619004295934
64 h	1.76303934510646	9.05134713991179	6.75910687742822

**Table S9: CARTESIAN COORDINATES of VBCMERI\_T+AsO<sub>2</sub><sup>-</sup>+As<sup>3+</sup> (ANGSTROM)**

1 as	5.76936054486570	9.54732637116840	9.45028765572732
2 cu	2.12262355964640	13.00618607480061	13.51117570035120
3 o	4.56012035157258	13.09029995540591	9.79642066182269
4 o	7.96458473809764	10.22154282665121	12.15384991149516
5 o	3.00535365735366	9.11341854354150	11.97061464895564
6 o	4.82459206387168	12.18956730838434	15.99156182631269
7 n	1.95880265908639	16.77331804196767	13.13333197628308
8 n	-1.51292462947590	12.01915233568043	13.06309429138391
9 c	0.88783352018964	18.06952010052535	15.34507335004113
10 c	2.23589521491948	18.06910139443109	11.06678854651452
11 c	-3.28057080932839	14.15316239492610	13.04654663251118
12 c	-2.53383406646232	5.17338138364300	13.51938247309310
13 c	4.15306136597842	14.78966202879116	7.93695154200772
14 c	1.60729261396588	7.05294421506816	12.53980153123123

15 c	-0.91551871417420	16.37049297081784	16.86197051078280
16 c	-1.06434328197424	7.35387554848951	12.96536022347780
17 c	3.14140194863933	17.23943644360559	8.59375725520432
18 c	-3.41558362465180	15.58909902917261	15.58820528072874
19 c	2.67725391849465	4.61477918825563	12.81933065457243
20 c	-2.44202138152759	9.74933347118623	12.93931778607020
21 c	1.17271744901506	2.51541249775044	13.40761591936378
22 as	7.80906924328552	11.27318191401789	15.35848330708769
23 c	2.87162586881618	19.08549112581857	6.65184454589250
24 c	-1.45583280018062	2.77307481232207	13.74284605448240
25 c	4.70418460296690	14.31851599070668	5.35301399272080
26 c	3.47661124177684	18.60137830210387	4.13204905081036
27 c	4.37573883390140	16.17833668729472	3.49926023274806
28 o	8.19327408265853	10.51938867922623	7.21830178054568
29 o	6.91238932091940	6.28149836306016	9.55839539095975
30 o	3.51075244675808	8.87359358475717	6.92631360639804
31 h	2.48883507602685	18.59703907402503	16.60875740507455
32 h	-0.06769933343360	19.86144069267261	14.76764148120663
33 h	1.63314110161219	20.08725219296182	11.09700180669532
34 h	-2.66190300706649	15.46305877680126	11.52430142542041
35 h	-5.22167596141547	13.49589916042830	12.55157413688543
36 h	-4.58452577413404	5.41857209394473	13.80751567483009
37 h	-1.39566938806196	17.39999459895602	18.63312793486272
38 h	0.14855229051995	14.65531132863021	17.46933804208109
39 h	-4.48104534589955	14.39826966600341	16.95835917255651
40 h	-4.59595436997945	17.29994657965823	15.25015478030435
41 h	4.72000469915168	4.40516407770431	12.52014668112511
42 h	-4.53724208461082	9.53917155806313	12.87051303061643
43 h	2.07359218361654	0.64608668848837	13.60733560950992
44 h	2.12678485540541	20.95731525375988	7.19069027784677
45 h	-2.64103020118172	1.12052482218992	14.18747432614366
46 h	5.42362487824098	12.45630467986697	4.81070030971905
47 h	3.23863495645836	20.07355023164657	2.67968509679414
48 h	4.84739010541615	15.71982363760357	1.52080916764689
49 h	9.73283602454773	9.62502556028976	7.77282692419035
50 h	6.04699534410412	5.40945290503150	8.15408626486762
51 h	1.79911527250552	9.17027131430785	7.59758303360922

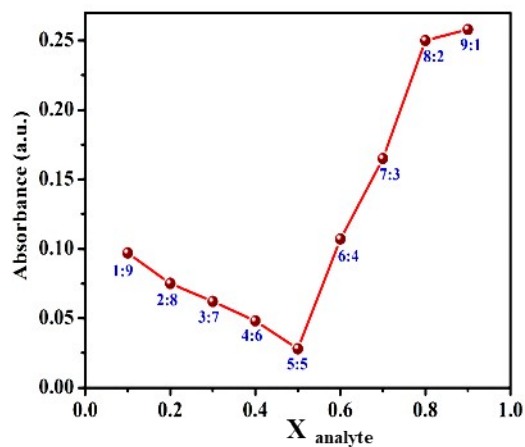


Fig.S4. Job's plot of VBCMERIC with  $\text{As}^{3+}$

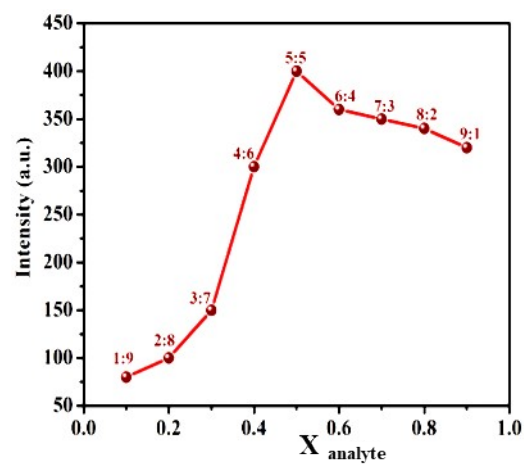


Fig.S5. Job's plot of VBCMERIC with  $\text{AsO}_2^-$

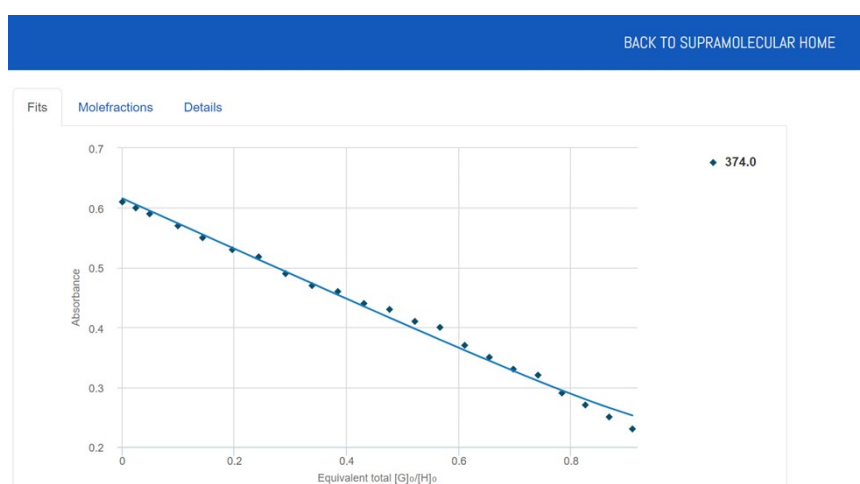
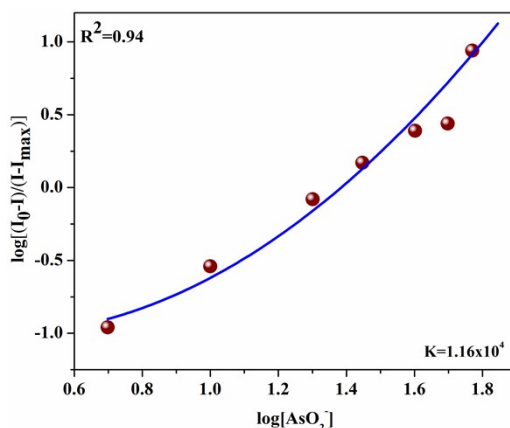


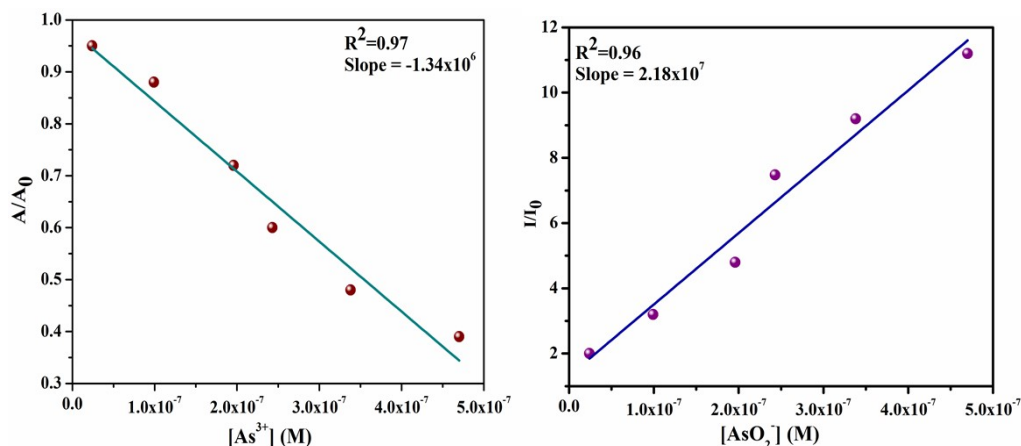
Fig.S6. Binding constant evaluation of VBCMERIC with  $\text{As}^{3+}$   
[\[http://supramolecular.org\]](http://supramolecular.org)  
 Binding constant =  $9.5 \times 10^5 \text{ M}^{-1}$



**Fig.S7.** Association constant plot for  $\text{AsO}_2^-$  with VBCMERI from emission titration

### Detection limit calculation

The detection limit (DL) has been calculated following UV-Vis titration for  $\text{As}^{3+}$  and PL titration for  $\text{AsO}_2^-$ . For LOD calculation, the concentration of  $\text{As}^{3+}$  and  $\text{AsO}_2^-$  were taken as  $10^{-5}$  M. The absorbance spectrum and emission spectrum of VBCMERI were repeated 5 times, and the standard deviation was measured. The limit of detection (LOD) is calculated from the following formula:  $\text{DL} = 3\sigma/k$ ;  $\sigma$  is the standard deviation of the blank solution of VBCMERI. Gradual emergence of new absorbance values during colorimetric quenching with  $\text{As}^{3+}$  and enhanced fluorogenic response with  $\text{AsO}_2^-$  are plotted against its concentration. The slope (k) is derived from these plots.

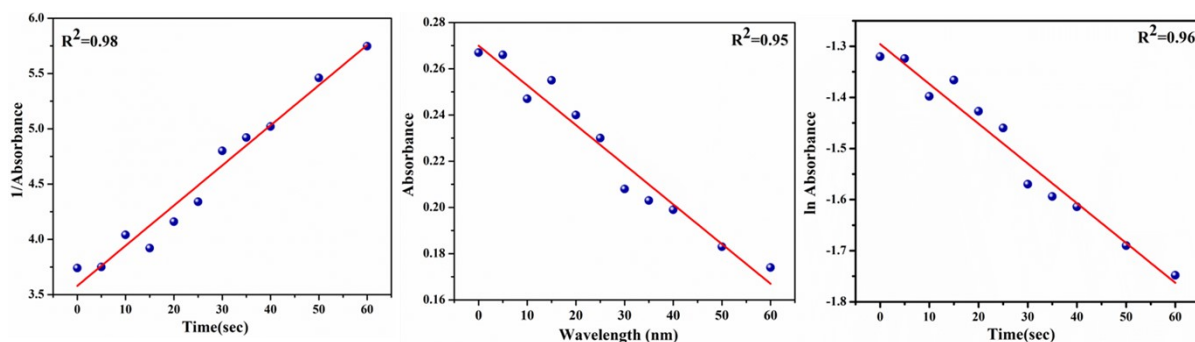


**Fig.S8.** The ratio of absorbance of VBCMERI with  $\text{As}^{3+}$  and (b) the Ratio of emission of VBCMERI with  $\text{AsO}_2^-$

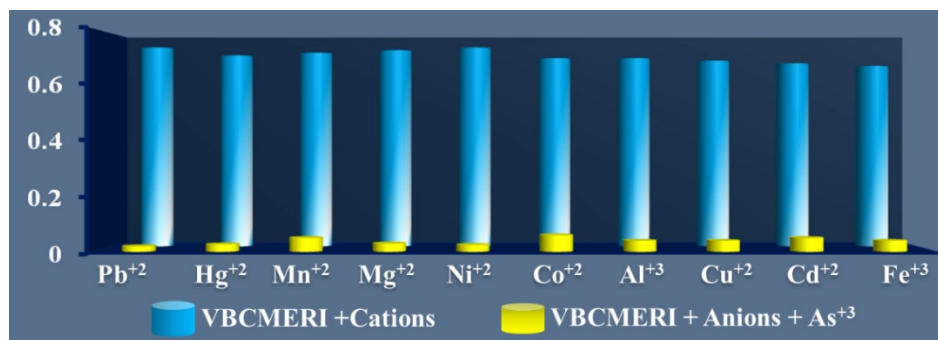
### Rate constant calculation

Rate constant of the host-guest interaction was calculated from UV-Vis spectroscopy. The sensor and the analytes were taken in similar concentration and the plots of absorbance vs. time were observed in a fixed wavelength. After those three graphs were plotted (i) Absorbance vs. time, (ii)  $\ln$  Absorbance

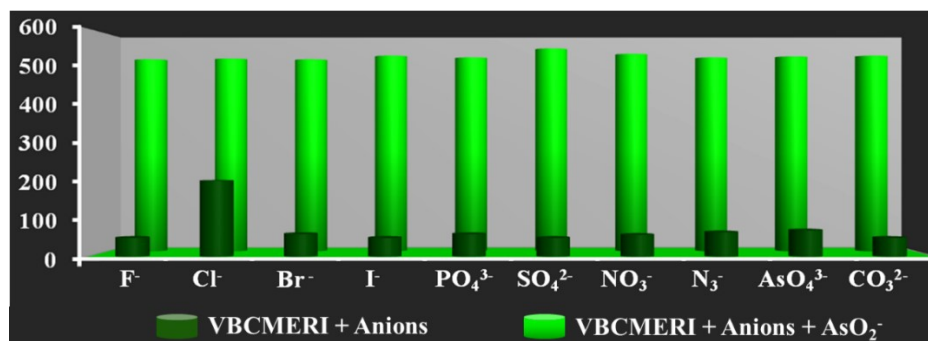
vs. time and (iii) 1/Absorbance vs. time. Among the three plots, the plot in which the R-value is more closed to 1 is chosen and accordingly the order of the reaction was known. Furthermore, the reaction rate was obtained from the slope of the specific plot.



**Fig.S9.** Plots of Absorbance vs. Time of VBCMEREI with  $As^{3+}$



**Fig.S10.a.** Interference of VBCMEREI with different cationic analytes in MeOH- $H_2O$



**Fig.S10.b.** Interference of VBCMEREI with different anionic analytes in MeOH- $H_2O$



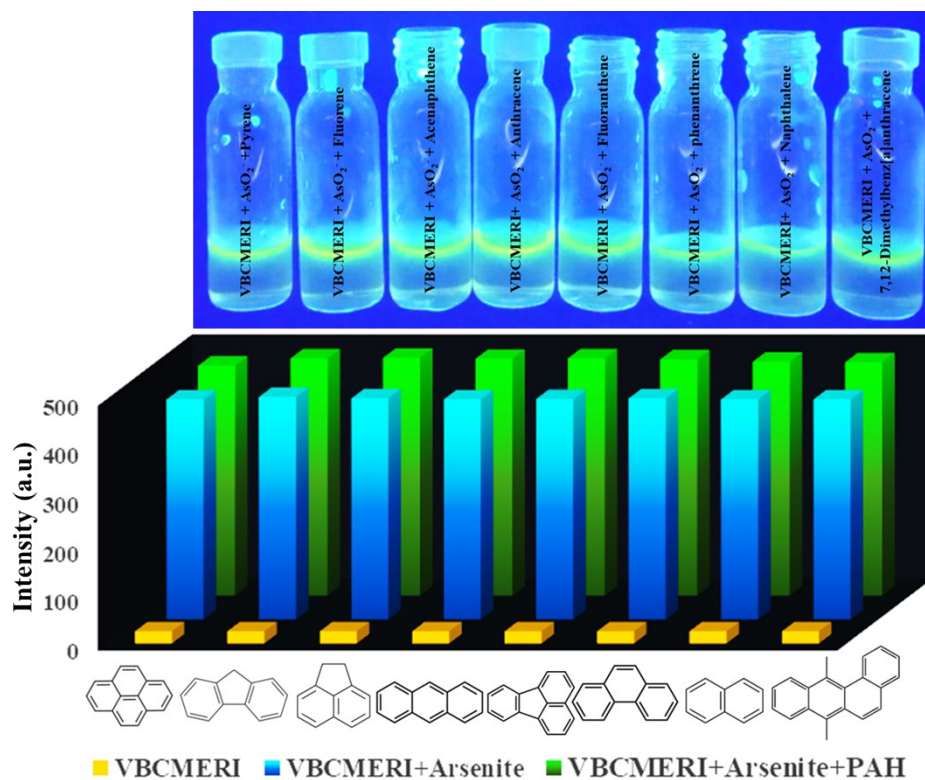


Fig.S10.c. Interference studies of VBCMERIC-AsO<sub>2</sub><sup>-</sup> with Poly-Aromatic Hydrocarbons (PAHs)

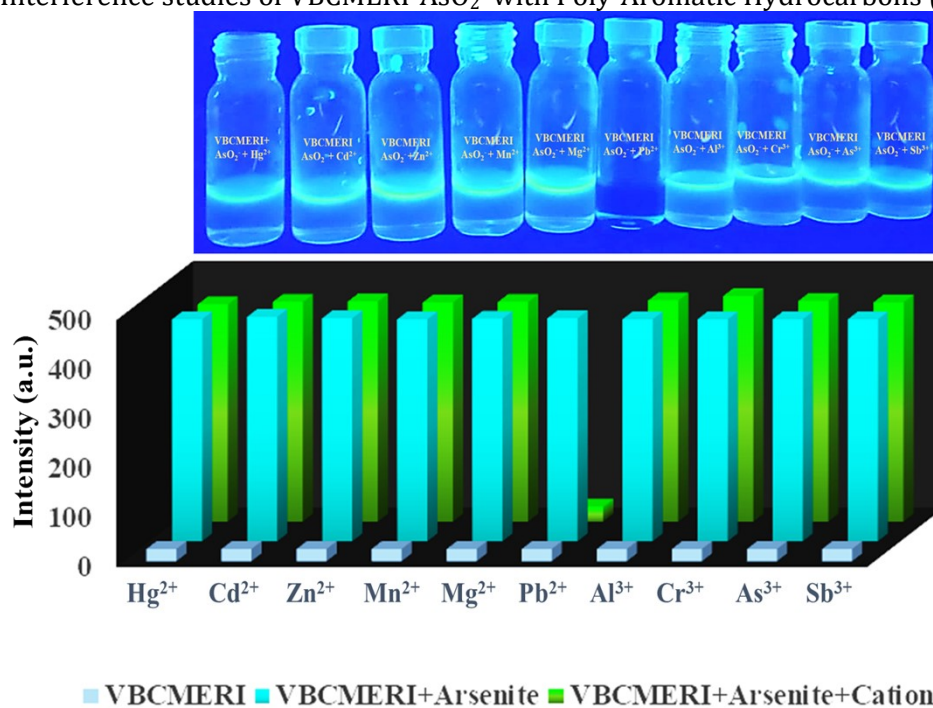


Fig.S10.d. Interference studies of VBCMERIC-AsO<sub>2</sub><sup>-</sup> with different divalent and trivalent metal cations

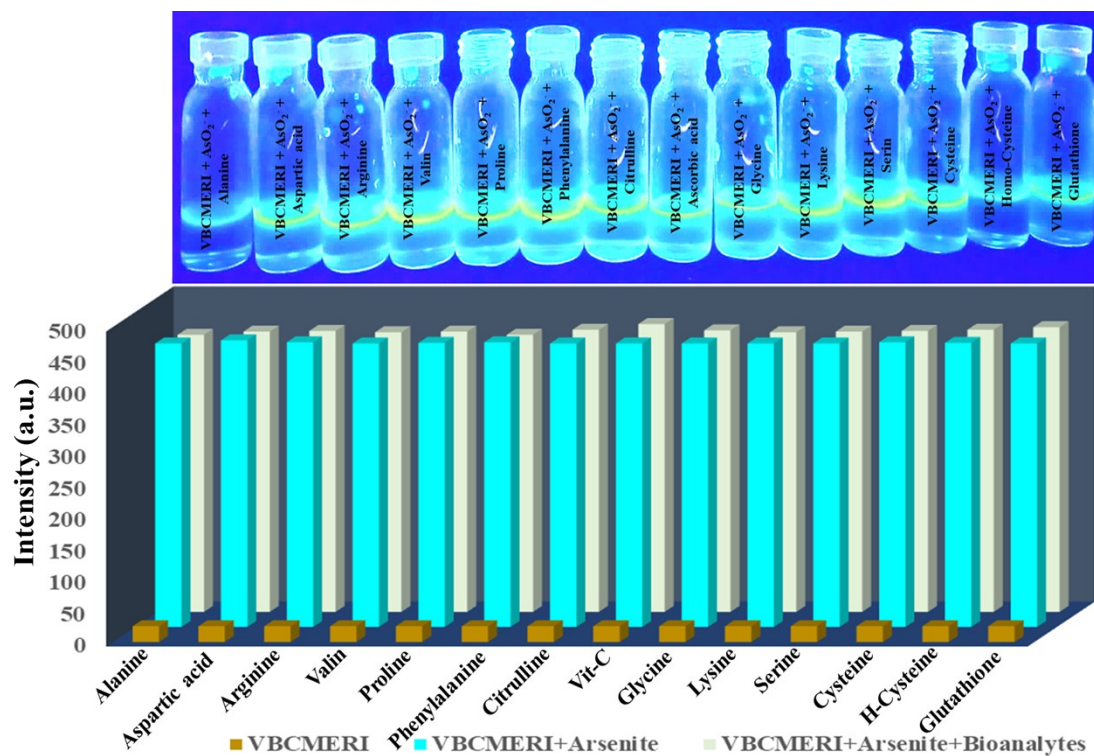


Fig.S10.e. Interference studies of VBCMERIC-AsO<sub>2</sub><sup>-</sup> with different bioanalytes

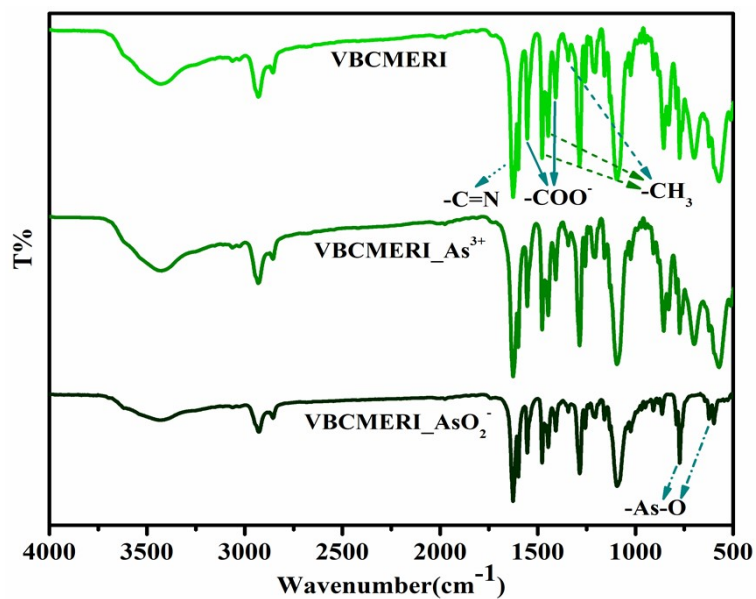


Fig.S11. FT-IR spectra of VBCMERIC, VBCMERIC+As<sup>3+</sup> and VBCMERIC + AsO<sub>2</sub><sup>-</sup> adduct

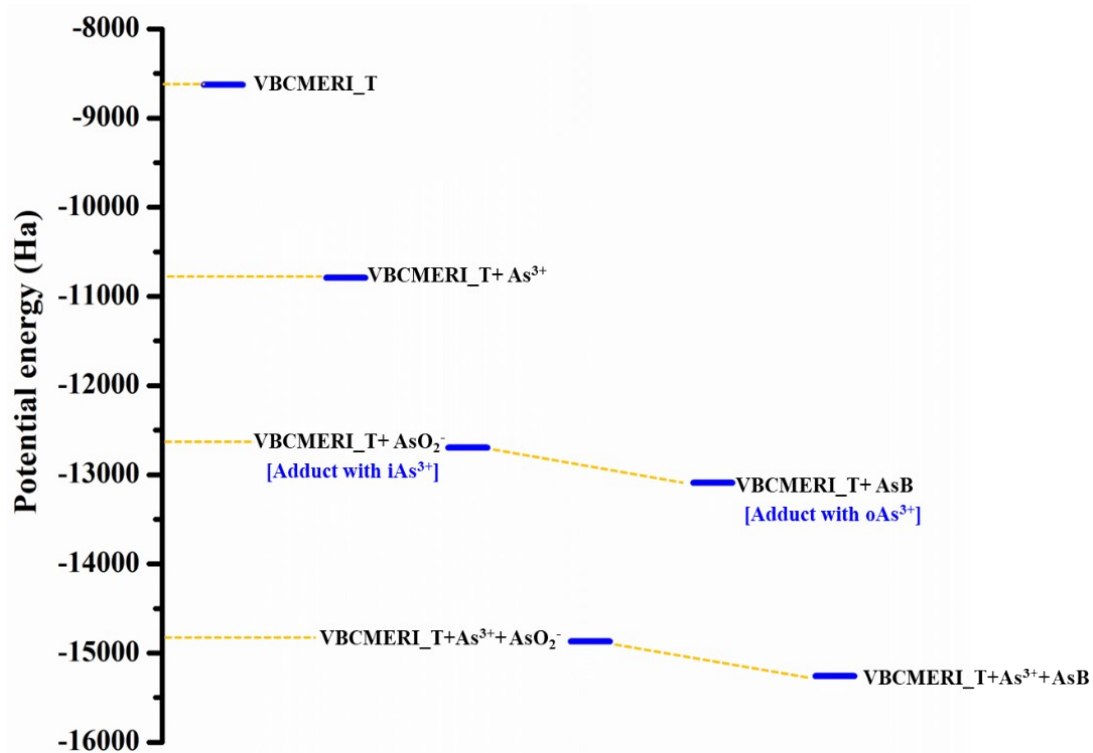
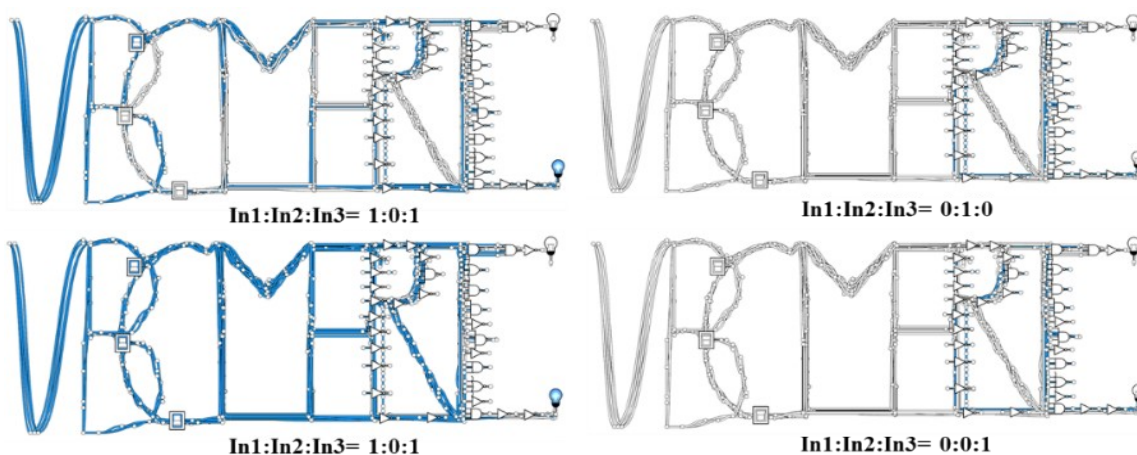


Fig.S12. Variation of P.E. with formation of VBCMEREI-arseno adducts

Complex_T	C	Cu	Mn	As	O	D.E.
VBCMEREI_T	23	1	1	0	7	-2.16 eV
VBCMEREI_T+As <sup>3+</sup>	23	1	0	1	7	-0.69 eV
VBCMEREI_T+AsO <sub>2</sub> <sup>-</sup>	18	1	1	1	7	-0.93 eV
VBCMEREI_T+AsO <sub>2</sub> <sup>-</sup> +As <sup>3+</sup>	18	1	0	2	7	-0.81eV
VBCMEREI_T+AsB	23	1	1	1	7	-2.39 eV
VBCMEREI_T+AsB+As <sup>3</sup>	23	1	0	2	7	-4.41eV

-Mn; +2As  
+As  
-5C; -Mn; +2As  
+As; -5C  
+As  
+As

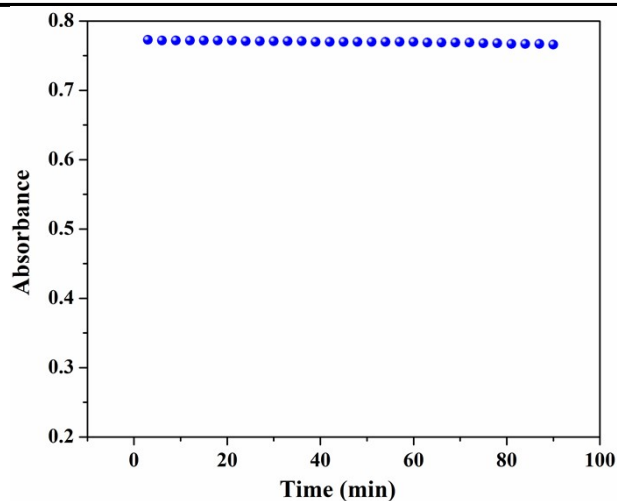
Fig.S13. Variation of D.E. with formation of VBCMEREI-arseno adducts



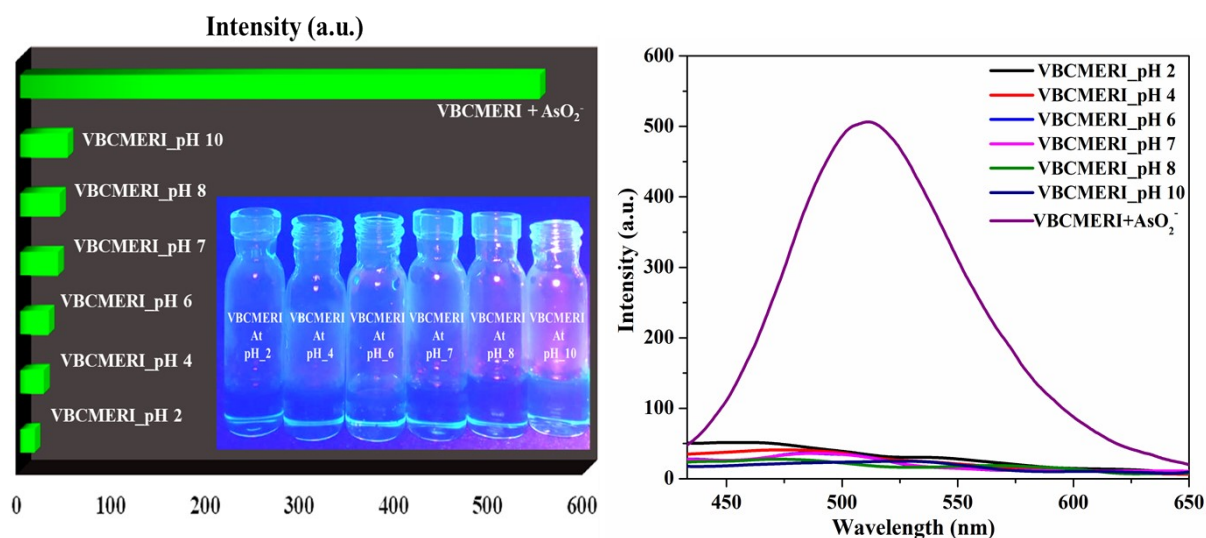
**Fig.S14.** Fabrication of the logic gate with outputs upon altering inputs of NAND–NOT–NOR logic functions for VBCMERI with  $\text{AsO}_2^-$  and  $\text{Pb}^{2+}$

**Table S10. Detection of aquifer-genic  $\text{As}^{3+}$  and  $\text{AsO}_2^-$  using VBCMERI**

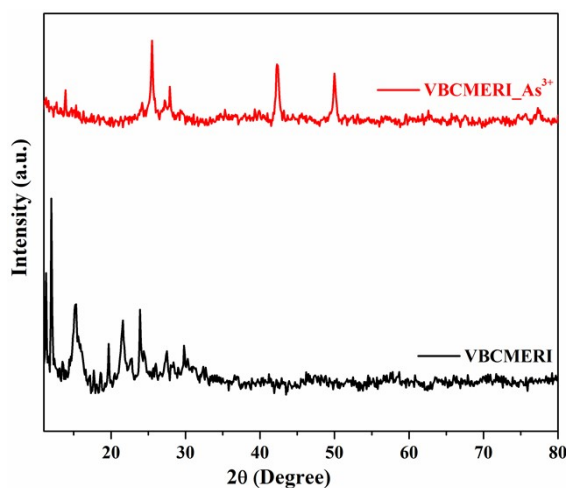
Location	$\text{As}^{3+}/\text{AsO}_2^-$ (ppb)	PL intensity
22.930247°N,88.730335°E	110.22	139.5
22.931100°N,88.730653°E	121.52	140
22.918097°N,88.720290°E	94.53	128.2
22.918097°N,88.720290°E	57.24	116
22.918094°N,88.720306°E	45.23	110
22.899767°N,88.735926°E	68.30	114.8
22.899767°N,88.735926°E	184.55	211.2
22.899767°N,88.735926°E	178.98	152.9
22.930267°N,88.730335°E	136.80	152.1
22.930267°N,88.730335°E	181.25	162



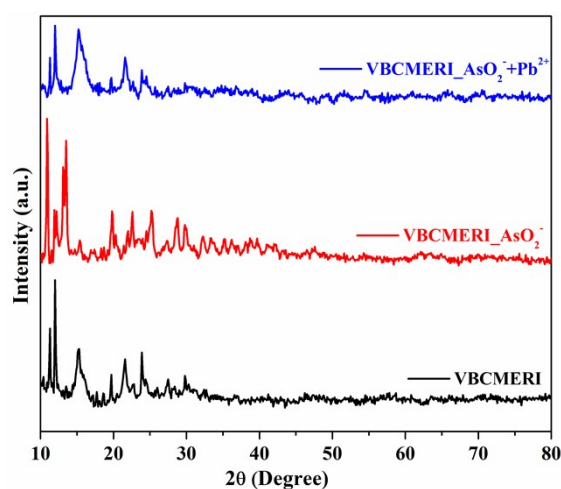
**Fig.S15.a.** Stability of  $\text{AsI}_3$  in  $\text{H}_2\text{O}$



**Fig.S15.b.** pH stability experiment of VBCMERIC probe: Left, bar diagram exhibiting comparative response of VBCMERIC at different pH and VBCMERIC- $\text{AsO}_2^-$  interaction (Inset, physical images of VBCMERIC at diverse pH); Right: Photoluminescence spectral response of VBCMERIC at different pH.



**Fig.S16.a.** Comparative X-Ray diffractogram of VBCMERIC and VBCMERIC+ $\text{As}^{3+}$



**Fig.S16.b.** Comparative X-Ray diffractogram of VBCMERIC, VBCMERIC+ $\text{AsO}_2^-$  and VBCMERIC+ $\text{AsO}_2^- + \text{Pb}^{2+}$



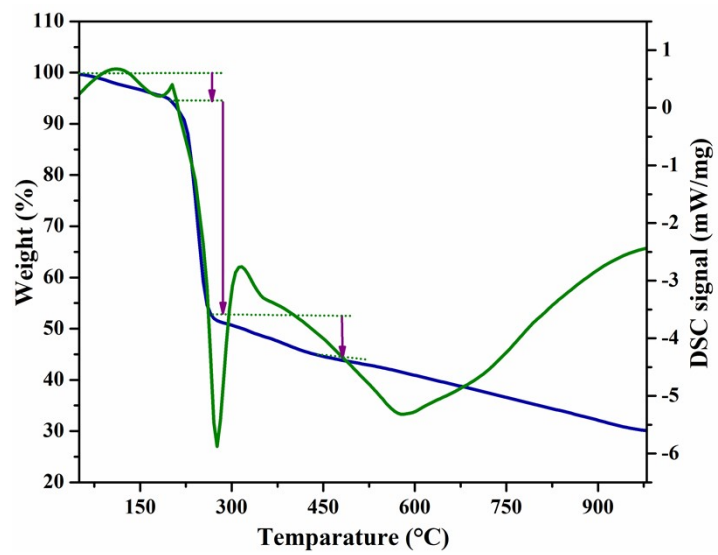


Fig.S17. TGA and DSC plot of VBCMERI probe