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Supporting Information

Axially Chiral Amino Acid Scaffold as an Efficient Fluorescent Discriminator of Methanol-Ethanol

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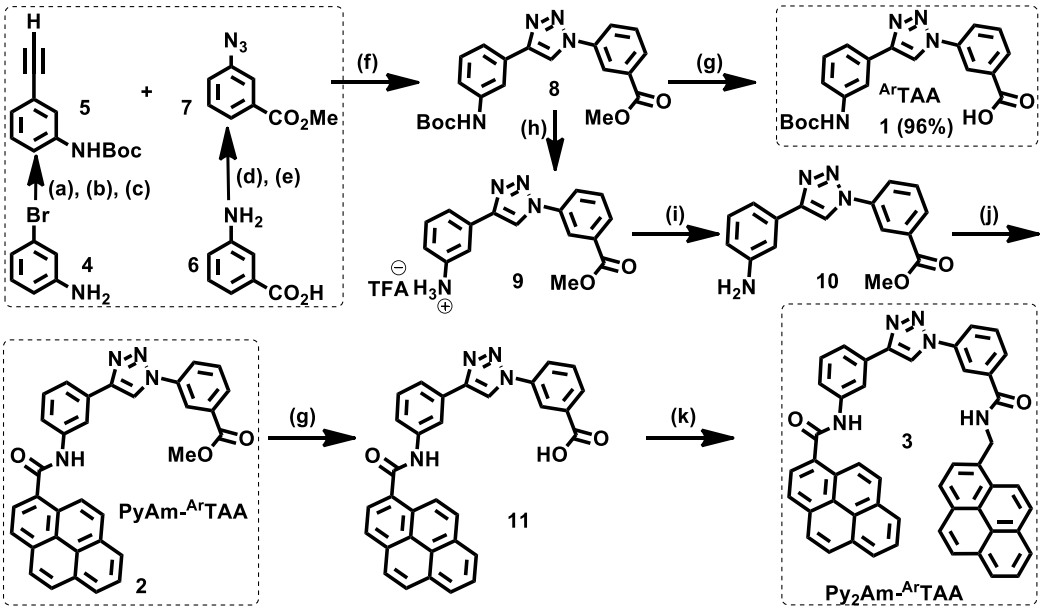
1. General Experimental Section (Materials and Methods)

All reactions were carried out under nitrogen atmosphere in flame-dried glassware, using a nitrogen filled balloon. Organic extracts were dried over anhydrous sodium sulfate. Solvents were removed in a rotary evaporator under reduced pressure. Silica gel (60- 120 mesh size) was used for the column chromatography. Reactions were monitored by TLC on silica gel 60 F254 (0.25). ^{1}H NMR spectra were recorded either at 400 MHz or at 600 MHz and ^{13}C NMR spectra were recorded either at 100 MHz or at 150 MHz (mentioned accordingly). Coupling constants (J value) were reported in hertz (Hz). The chemical shift were shown in ppm downfield form tetramethylsilane, using residual chloroform (δ = 7.26 in ^{1}H NMR, δ = 77.23 in ^{13}C NMR), DMSO (δ = 2.5 in ^{1}H NMR, δ = 39.5 in ^{13}C NMR), as an internal standard. Mass spectra were recorded with a HR mass spectrometer and data analysed by using built-in software. IR spectra were recorded in KBr on a FT-IR spectrometer.

2. Synthetic Schemes



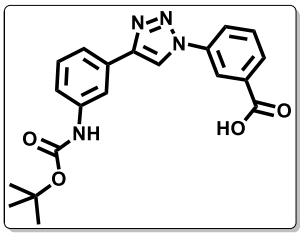
Reagents and Condition: (a) $(Boc)_2O$, THF, NaH, reflux, 12 h; (b)TMS-acetylene, $PdCl_2(PPh_3)_2$, CuI, Benzene : ^{n}Butyl amine (2:1), 70 °C, 6h; (c) TBAF, THF, r.t, 1 h; (d) $SOCl_2$, methanol, reflux, 3h; (e) $NaNO_2$, HCl/NaN_3, 0 °C, 2 h; (f) $CuSO_4$, NaAsc, Et_3N, THF: H_2O (4:1), rt, 12 h; (g) LiOH, THF:H_2O (5:1), rt, 1 h; (h) DCM :TFA(1:1), rt, 1 h; (i) aq. Et_3N; (j) 3-Pyrene carboxylic acid, MsCl, *N*-methyl imidazole, DCM, 0-50 °C, 6 h; (k) Pyren-1-ylmethanamine, EDC.HCl, DMAP, DMF, 0 °C - rt, 6h.

Scheme S1: Synthetic scheme for the triazolyl aromatic amino acid scaffold (**1**,**^{Ar}TAA**) and its mono and di-pyreneamide derivatives (**2**, **PyAm-^{Ar}TAA; 3**, **Py$_2$Am-^{Ar}TAA**).

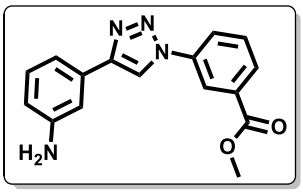
3. Synthetic route of aromatic triazolyl amino acid scaffold 1 and its pyrenyl derivatives (^{Ar}TAA)

3.1. ***Synthesis of methyl 3-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1H-1,2,3-triazol-1-yl)benzoate*** **(8):** The compound **8** was synthesized as our previous published protocol.

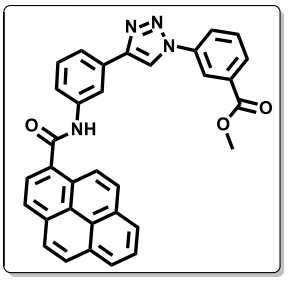
3.2. ***Synthesis of 3-(4-(3-((tert-butoxycarbonyl)amino)phenyl)-1H-1,2,3-triazol-1-yl)benzoic acid*** **(1):**To a solution of the starting material **8**, (250 mg, 0.65 mmol) in THF : H_2O = 5 : 1 (6 ml), lithium hydroxide (1.5 equivalent) was added at 0 ^oC. The reaction mixture was stirred for about 3-4 hour until starting material was fully consumed. Reaction was monitored by TLC. After completion of the reaction, solvent was dried by a rotary evaporator. Then water (4-5 ml) was added to the reaction mixture and cooled to 0 ^oC. The dilute acetic acid was added to the reaction mixture to adjust pH~ 3 to 4. The reaction mixture was extracted with EtOAc. The combined organic layers were dried over Na_2SO4. Title compound **9** (222 mg, 0.58 mmol) was isolated as a white solid material in pure form by column chromatography (Si-gel, PE :EtOAc = 1:2).. Yield 93%. ^{1}H NMR (d_6-DMSO; 400 MHz) δ 1.47 (9H, s); 7.36 (2H, s); 7.51 (1H, s); 7.75 (1H, t, J = 7.6 Hz); 8.04 (1H, d, J = 6.8 Hz), 8.16 (1H, s); 8.08 (1H, d, J = 8.0 Hz); 8.46 (1H, s); 9.33 (1H, s); 9.47 (1H, s); ^{13}C NMR (d_6-DMSO; 100 MHz) δ 28.4, 79.6, 115.3, 118.5, 119.9, 120.1, 120.6, 120.7, 124.4, 129.5, 130.8, 132.9, 137.1, 140.4, 147.9, 153.2, 166.7. HRMS calcd for $C_{20}H_{21}N_4O_4$ $[M + H]^+$ 379.1557, found 379.1558.



3.3. ***Synthesis of methyl 3-(4-(3-aminophenyl)-1H-1,2,3-triazol-1-yl)benzoate*** **(10):** The compound **8** was dissolved in dry DCM and cooled to 0 °C. Then equal amount of TFA (1 ml) was added and allowed to warm to room temperature. Stirring was continued at room temperature until the starting material was fully consumed (TLC monitoring). The reaction mixture was evaporated *in vacuo*. The product **9** (as a TFA salt) was obtained in quantitative yield. To get free amine, water (4-5 ml) was added and cooled to 0 ^oC. Then dilute aq.Et_3N was added to the reaction mixture to neutralize excess TFA and adjusted the pH~ 8. Then the reaction mixture was extracted with EtOAc. The combined organic layers were dried over Na_2SO_4 and evaporated *in vacuo* to yield the crude product **10** in quantitative yield and used for next step.

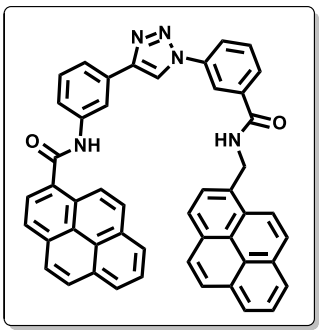


***Synthesis of methyl 3-(4-(3-(pyrene-1-carboxamido)phenyl)-1H-1,2,3-triazol-1-yl)benzoate* (2):** In a dry round bottom flask, 1-pyrene carboxylic acid (125 mg, 0.5 mmol) dissolved in 6 ml dry DCM was cooled to 0 ^{o}C in an ice bath. Reaction mixture was basified with N-methyl imidazole (119 µl, 1.5 mmol) and mesyl chloride (38 µl, 0.5 mmol) was added



under nitrogen atmosphere. After 15 minute, ice bath was removed to attain room temperature. The free amine **10** (132 mg (0.45 mmol) dissolved in 2 ml dry DCM was added to the reaction mixture and refluxed at 50 ^{o}C overnight. After consumption of amine the solvent was dried by rotary evaporator and partitioned between EtOAc and aqueous $NaHCO_3$ solution (20 ml each). The organic layer was washed with brine solution. Pure product **2** (120 mg, 0.229 mmol) was isolated by column chromatography (Si-gel, PE :EtOAc = 2:1). Yield 54 %. IR (KBr) 3248, 3043, 2952, 2850, 1724, 1655, 1591, 1527, 1248, 1041, 849, 756 cm^{-1}. ^{1}H NMR ($CDCl_3$ and d_6-DMSO mix (20%); 400 MHz) δ 3.73 (3H, s); 7.25 (1H, t, *J* = 7.6 Hz); 7.40 (1H, t, *J* = 7.6 Hz); 7.52 (1H, d, *J* = 8 Hz); 7.65 (1H, d, *J* = 8 Hz); 7.82 (1H, d, *J* = 2.8 Hz); 7.85 (3H, m); 7.92 (2H, dd, *J* = 4.4 Hz); 8.02 (4H, ddd, *J* = 8 Hz, 4.4 Hz, 3.2 Hz); 8.33 (2H, d, *J* = 7.6 Hz), 8.39 (1H, d, *J* = 9.6 Hz); 8.57 (1H, s); 10.11 (1H, s); ^{13}C NMR ($CDCl_3$ and d_6-DMSO mix (20%); 100 MHz) δ 52.2, 117.2, 118.8, 119.9, 120.5, 121.1, 124.2, 124.4, 125.2, 125.5, 126.3, 127.1, 128.3, 128.5, 129.2, 130.0, 130.3, 130.7, 131.4, 137.2, 139.8, 147.9, 165.4, 165.6. HRMS calcd for $C_{33}H_{23}N_4O_3$ ($[M + H]^+$) 523.1764, found 523.1742.

3.4. ***Synthesis of N-(3-(1-(3-((pyren-1-ylmethyl)carbamoyl)phenyl)-1H-1,2,3-triazol-4-yl)phenyl)pyrene-1-carboxamide* (3):** In a dry round bottom flask, starting material **11** (30 mg, 0.059 mmol) in 3 ml dry DMF was cooled to 0 ^{o}C in an ice bath and EDC.HCl



(0.088 mmol) and DMAP (0.177 mmol) was added under nitrogen atmosphere. After 15 minute of stirring, pyren-1-ylmethanamine was added to the reaction mixture and stirred for half an hour at 0 ^{o}C. Then the ice bath was removed and the reaction mixture was stirred for about 18 hour. After completion of the reaction, it was partitioned between EtOAc and aqueous $NaHCO_3$ solution (10 ml each). The organic layer was washed with brine solution. Pure product **3** (22 mg, 0.03 mmol) was isolated by column chromatography (Si-gel, $CHCl_3$:MeOH = 10 : 1). Yield 52 %. IR (KBr) 3421, 3264, 3042, 2922, 2845, 1724, 1643, 1533, 1482, 1340, 1306, 1036, 845, 709 cm^{-1}.^{1}H NMR (d_6-DMSO; 600 MHz) δ 5.28 (2H, d, *J* = 6 Hz); 7.52 (1H, t, *J* = 7.8 Hz); 7.77-7.67 (2H, m); 7.83 (1H, d, *J* = 8 Hz); 8.05 (2H, dd, *J* = 15.1 Hz, 7.6); 8.19-8.10 (5H, m); 8.28 (8H, ddd, *J* = 18.9, 14.4, 8.6 Hz); 8.33-8.43 (3H, m); 8.47-8.56 (3H, m); 8.61 (1H, s); 9.37 (1H, s), 9.49 (1H, t, *J* = 5.4 Hz); 10.9 (1H, s); ^{13}C NMR (d_6-DMSO; 150 MHz) δ 41.3, 116.9, 119.0, 119.9, 121.2, 122.8, 123.2, 123.7, 123.8, 124.0, 124.1, 124.5, 124.8, 125.2, 125.3, 125.5, 125.8, 126.1, 126.3, 126.7, 126.9, 127.1, 127.3, 127.4, 127.7, 127.9, 128.2, 128.6, 129.6, 130.2, 130.3, 130.8, 130.9, 131.7, 131.9, 132.6, 135.9, 136.7, 140.1, 147.5, 165.2, 167.9. HRMS calcd for $C_{49}H_{32}N_5O_2$ ($[M + H]^+$) 722.2550, found 722.2540.

4. Study of Photophysical Property

4.1.*UV-visible & fluorescence measurements method*

All the UV –visible spectra of our synthesized compounds (10 µm) were measured in different solvents and different alcohol using UV-Visible spectrophotometer with cell path length 1 cm at 25 ^{o}C. All the sample solutions were prepared before an hour for the experiment. Fluorescence spectra were measured using a fluorescence spectrophotometer at 25 °C using 1 cm path length cell .All the sample solutions with same concentration as described in UV measurement experiments. The excitation wavelengths were set at λ^{abs}_{max}. Time resolved fluorescence decays were measured using time resolved fluorescence spectrophotometer. The fluorescence quantum yields (Φ_f) were determined using quinine sulphate as a reference with the known Φ_f= 0.54 in 0.1 molar solution in sulphuric acid.

4.2.*UV-visible and Fluorescence Spectra of* 1(^{Ar}TAA)

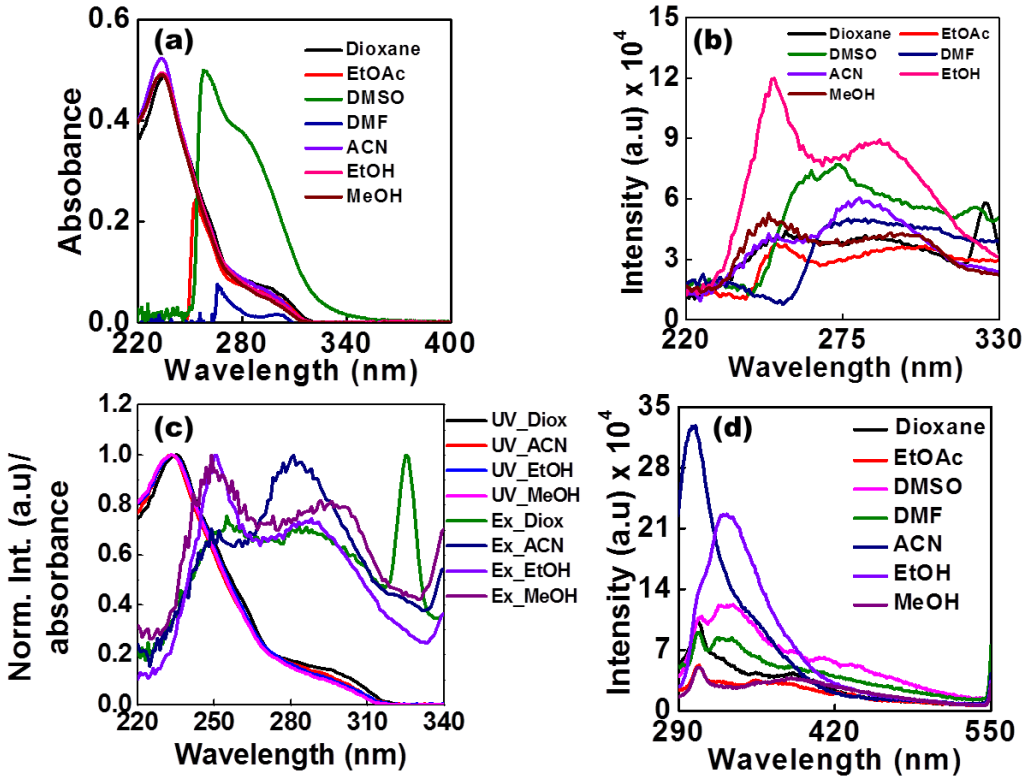


Figure S1. (a)UV-Visible (b)excitation, (c) normalised absorbance and excitation spectra, (d) fluorescence emission spectra of the **TriazolylAromatic Amino Acid Scaffold 1(^{Ar}TAA)**in different solvents [10 µM, r.t.; $\lambda_{ex} = \lambda_{max} \approx 280$ nm in each solvent].

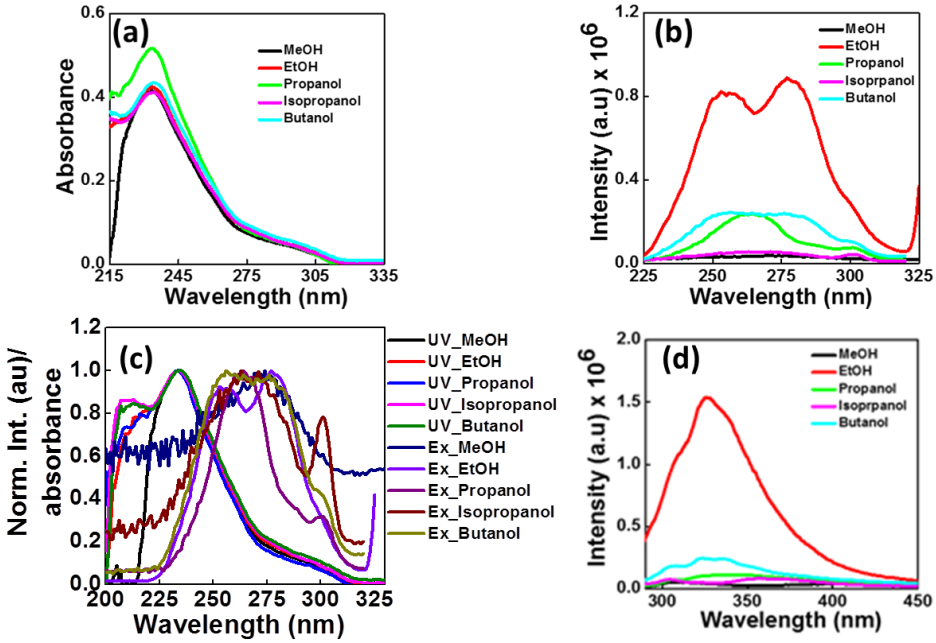


Figure S2. (a)UV-Visible (b)excitation, (c) normalised absorbance and excitation spectra, (d) fluorescence emission spectra of the **Triazolyl Aromatic Amino Acid Scaffold 1(**^{Ar}**TAA)**in different alcohols [10 µM, r.t.; $\lambda_{ex} = \lambda_{max} \approx 280$ nm in each solvent].

4.2.1. *Titration of Ethanol in Methanol solvent*

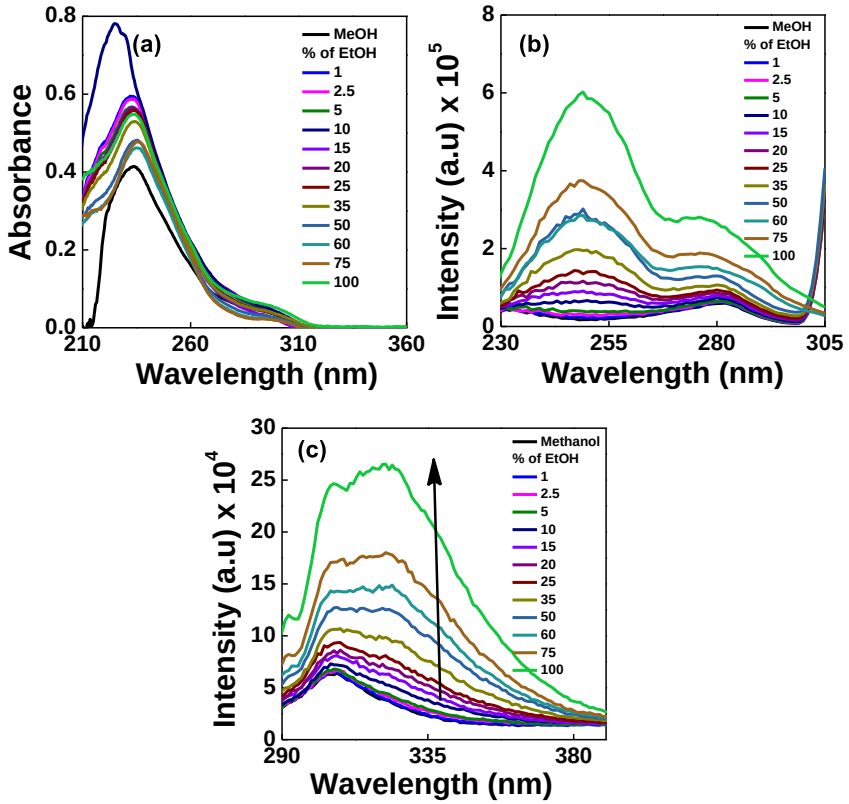


Figure S3. (a)UV-Visible (b)excitation and (c)fluorescence emission spectra of^{Ar}**TAA(1)**in methanol with increasing volume of ethanol. [10 µM, r.t.; $\lambda_{ex} = \lambda_{max} \approx 280$ nm in each solvent].

4.2.2. *Titration of Ethanol in Dioxane solvent*

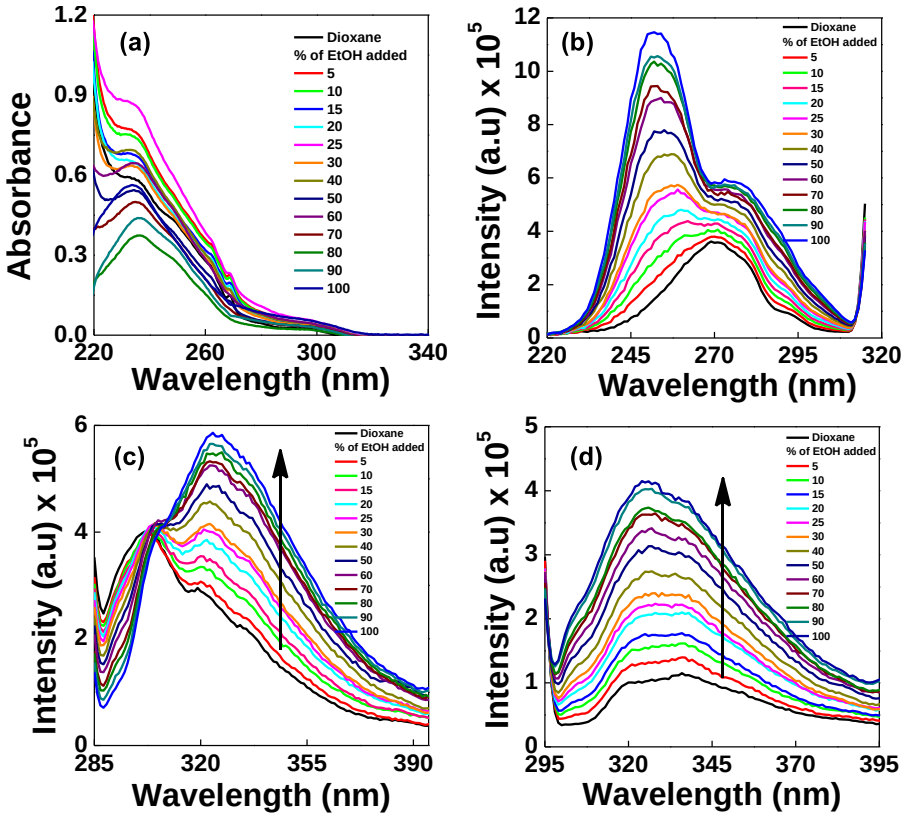


Figure S4. (a)UV-Visible (b) excitation (λ_{ex} = 330 nm) and fluorescence emission spectra (c) λ_{ex} = 280 nm and (d) λ_{ex} = 290 nm of **^{Ar}TAA (1)**in Dioxane with increasing percentage of ethanol [10 µM, r.t.].

4.3.*UV-visible and Fluorescence Spectra of 2 (PyAm-^{Ar}TAA) in Different Alcohol.*

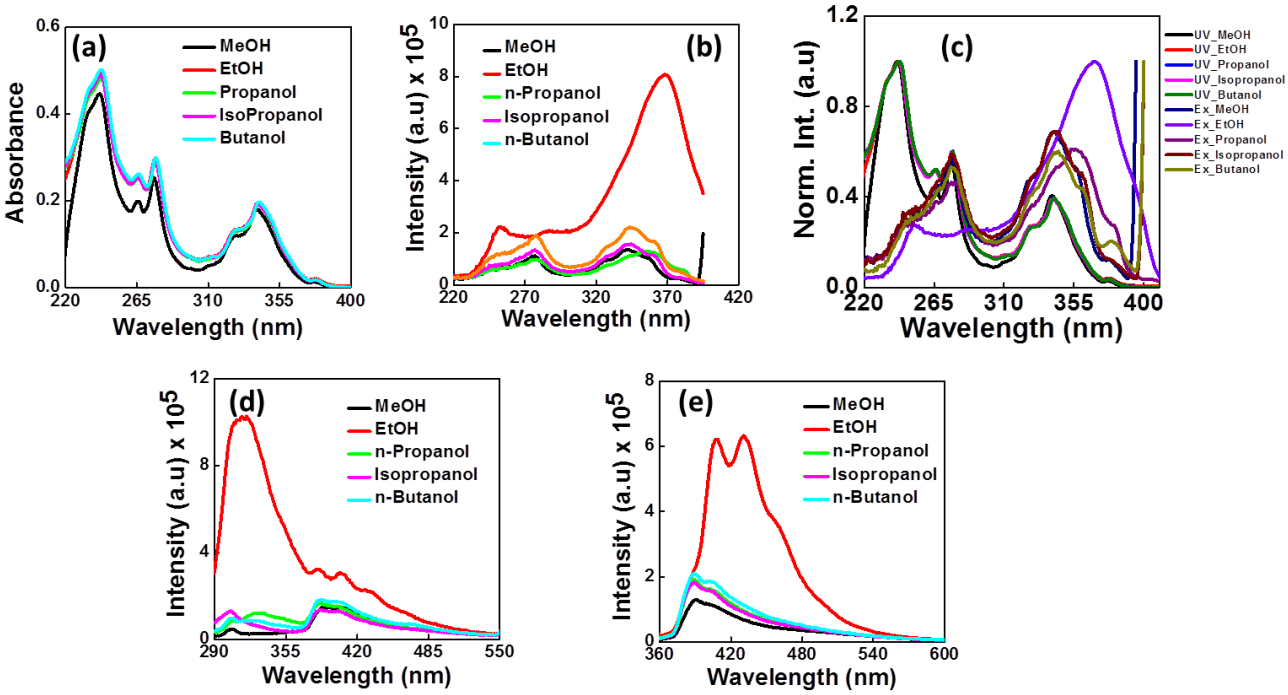


Figure S5. (a)UV-Visible (b) excitation (λ_{ex} = 410-430 nm), (c) normalised absorbance and excitation spectra, and fluorescence emission spectra at (d) λ_{ex}= 280 nm and (e) at λ_{ex}= 350 nm of the mono-pyrene derivative of triazolyl aromatic amino acid scaffold **2**, **PyAm-^{Ar}TAA** in different alcohol [10 µM, r.t.].

4.3.1. *Titrationof Ethanol in Methanol solvent*

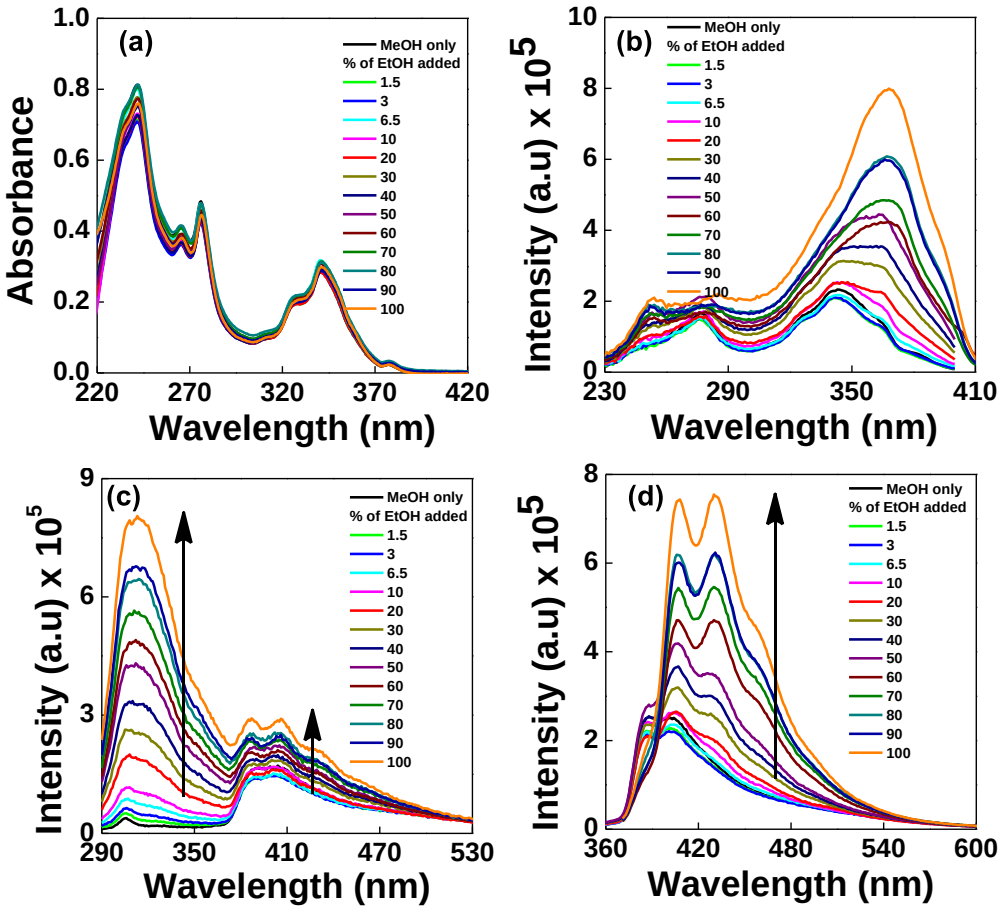


Figure S6. (a)UV-Visible (b) excitation (λ_{ex} = 410-430 nm) and fluorescence emission spectra (c) λ_{ex} = 280 nm and (d) λ_{ex} = 350 nm of the mono-pyrene derivative of triazolyl aromatic amino acid scaffold **2, PyAm-^{Ar}TAA**in methanol with increasing volume of ethanol.[10 µM, r.t.].

4.4. *UV-visible and Fluorescence Spectra of di-pyrene derivative of our scaffold3 (Py_2Am-^{Ar}TAA) in Different Alcohol.*

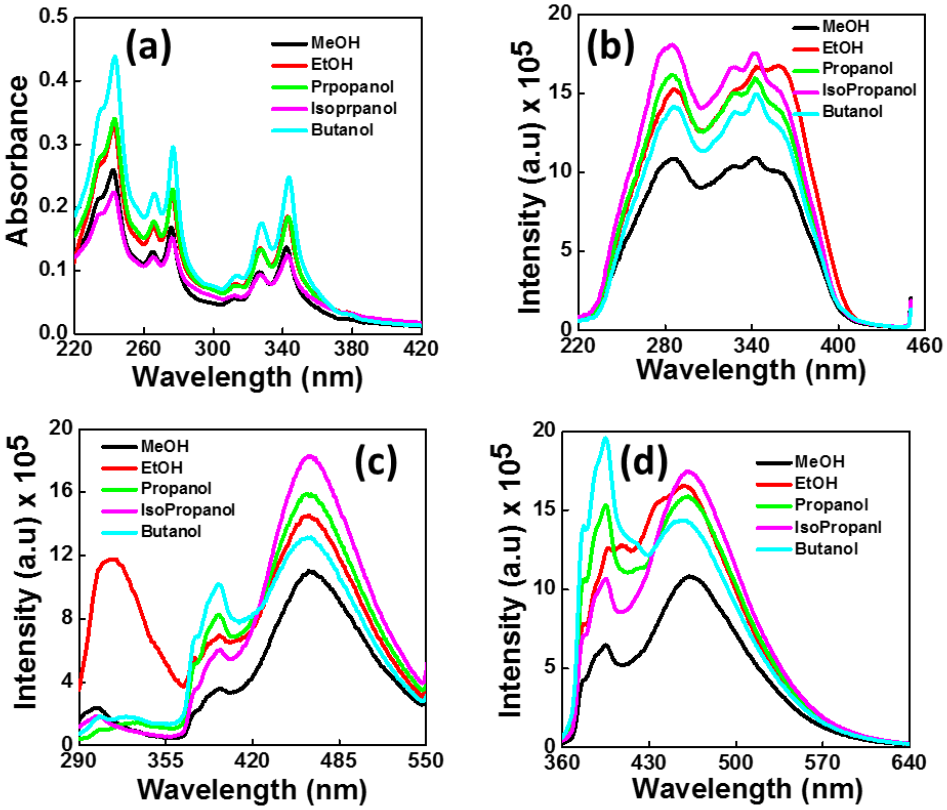


Figure S7. (a)UV-Visible (b) excitation (λ_{ex} = 460 nm) and fluorescence emission spectra (c) λ_{ex} = 280 nm and (d) λ_{ex} = 350 nm of the di-pyrene derivative of triazolyl aromatic amino acid scaffold **3** (**Py_2Am-^{Ar}TAA**)in different alcohol [10 µM, r.t.].

4.4.1. *Titration of Ethanol in Methanol solvent*

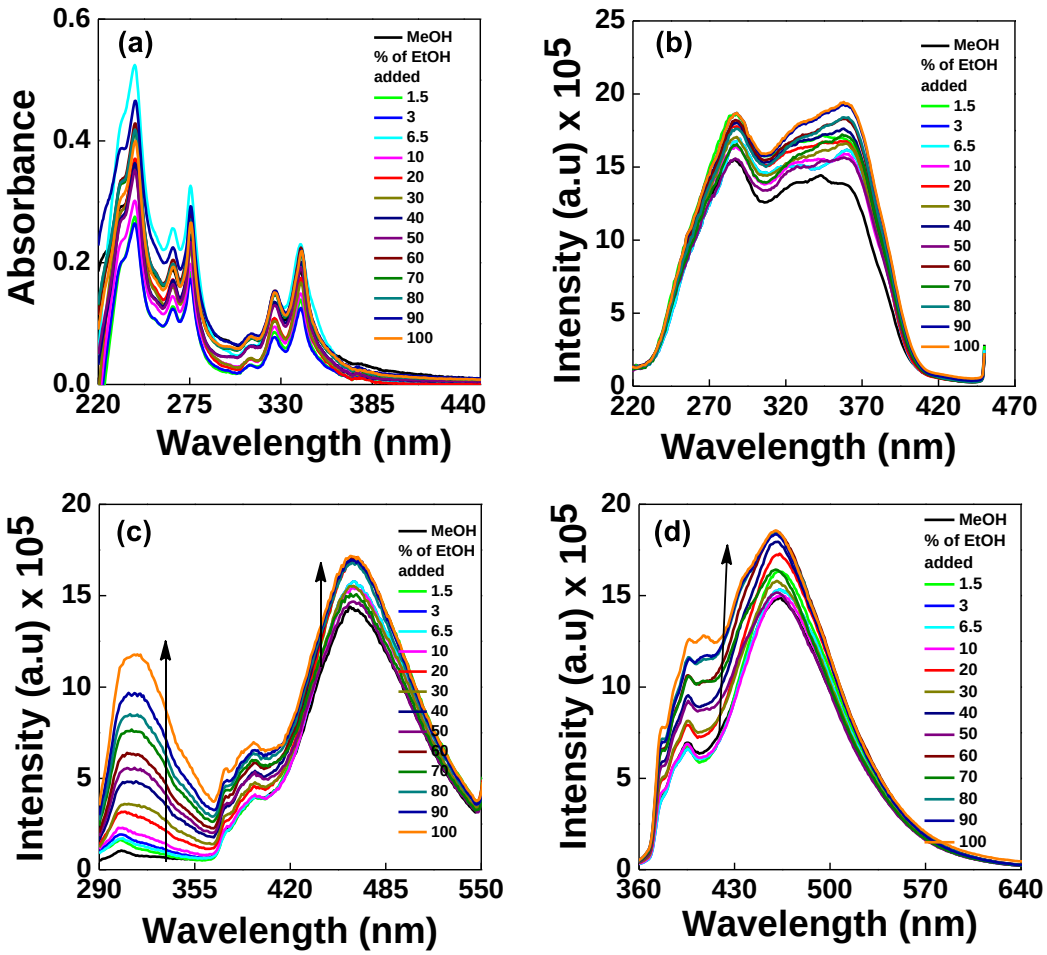


Figure S8. (a)UV-Visible (b) excitation (λ_{ex} = 460nm) and fluorescence emission spectra (c) λ_{ex} = 280 nm and (d) λ_{ex} = 350 nm of the di-pyrene derivative of triazolyl aromatic amino acid scaffold **3 (Py_2Am-^{Ar}TAA)**in methanol with increasing volume of ethanol.[10 µM, r.t.].

5. Photophysical Properties Summary

Table S1: Summary table of photophysical properties of the **1(^{Ar}TAA)**

Entry	Solvents	Relative polarity	UV-Vis & Fluorescence			
			λ_{max}^{abs} (nm)	ε_{max}x 10^2	λ_{max}^{fl} (nm)	Φ_f
1(^{Ar}TAA)	MeOH	0.762	287	63	305	0.004
	EtOH	0.654	289	72.7	326	0.07
	Propanol	0.617	284	69.8	342	0.008
	Isopropanol	0.546	279	73.8	364	0.005
	Butanol	0.586	288	82.1	330	0.012

Table S2: Summary table of photophysical properties of the **2(PyAm-^{Ar}TAA)**

Entry	Solvents	Relative polarity	UV-Vis & Fluorescence			
			λ_{max}^{abs} (nm)	ε_{max}x 10^2	λ_{max}^{fl} (nm)	Φ_f
2 (PyAm-^{Ar}TAA)	MeOH	0.762	275, 341	163	305, 401	0.004
	EtOH	0.654	276, 342	180	318, 408, 432	0.030
	Propanol	0.617	276, 341	178	329, 390, 401	0.01
	Isopropanol	0.546	276, 342	179	303, 388, 400	0.009
	Butanol	0.586	276, 341	187	316, 389, 404	0.01

Table S3: Summary table of photophysical properties of the **3 (Py_2Am-^{Ar}TAA)**

Entry	Solvents	Relative polarity	UV-Vis & Fluorescence			
			λ_{max}^{abs} (nm)	ε_{max}x 10^2	λ_{max}^{fl} (nm)	Φ_f
3 (Py_2Am-^{Ar}TAA)	MeOH	0.762	275, 326, 342	109	303, 394, 462	0.06
	EtOH	0.654	276, 326, 342	159	316, 395, 461	0.12
	Propanol	0.617	276, 327, 343	169	330, 394, 462	0.10
	Isopropanol	0.546	276, 327, 343	111	303, 395, 463	0.12
	Butanol	0.586	276, 327, 342	230	326, 394, 462	0.081

Table S4: Summary table of % of enhancement of intensity and quantum yield from MeOH to EtOH of our compound.

Entry	**% of enhancement intensity from MeOH to EtOH**						
	λ_{ex}= 280 nm	**λ_{em}**			**λ_{ex}=350 nm**	**λ_{em}**	
		330 nm	430 nm	465 nm		430 nm	460 nm
1, ^{Ar}TAA		1430	-----	-----		-----	-----
2, PyAm-^{Ar}TAA		2260	114	-----		386	-----
3, Py_2Am-^{Ar}TAA		1173	98	39		104	55
% of enhancement $\Phi_f$from MeOH to EtOH							
1, ^{Ar}TAA	**λ_{ex}= 280 nm**	1650	-----	-----	**λ_{ex}=350 nm**	-----	-----
2, PyAm-^{Ar}TAA		1600	200	-----		250	-----
3, Py_{2Am}-^{Ar}TAA		925	520	53		60	42

6. Life time table and Trace

Table S5: Summary table of fluorescence lifetimes of the **1 (^{Ar}TAA), 2 (PyAm-^{Ar}TAA) and3 (Py$_2$Am-^{Ar}TAA)**in different alcohol.

Entry	Solvents	Φ_f	λ [nm]	τ_1 [ns]	τ_2[ns]	<τ>[ns]	k_f [$10^8 s^{-1}$]	k_{nr}[10^8 s^{-1}]	χ^2
λ_{ex} = 290 nm									
1, ^{Ar}TAA	**MeOH**	0.004	330	3.48 (100%)	------	3.48	0.011	2.86	0.93
	10% EtOH	0.005	330	1.14 (31%)	5.01 (69%)	3.8	0.013	2.61	0.95
	50% EtOH	0.008	330	2.0 (24%)	6.44 (75%)	5.39	0.014	1.83	1.04
	90% EtOH	0.02	330	3.59 (50%)	8.59 (50%)	5.92	0.033	1.65	1.02
	Only EtOH	0.07	330	3.65 (49%)	8.85 (51%)	6.21	0.112	1.49	1.03
1, ^{Ar}TAA	**Dioxane**	0.004	330	4.05 (100%)	------	4.05	0.009	2.36	0.94
	10% EtOH	0.006	330	1.84 (42%)	6.82 (58%)	4.85	0.012	2.04	1.08
	50% EtOH	0.017	330	3.46 (40%)	8.14 (60%)	6.37	0.026	1.54	1.03
	90% EtOH	0.03	330	3.26 (42%)	8.85 (58%)	6.48	0.046	1.49	1.05
	Only EtOH	0.07	330	3.65 (49%)	8.85 (51%)	6.21	0.112	1.49	1.03
2 (PyAm-^{Ar}TAA)	**MeOH**	0.001	330	3.73 (100%)	------	3.73	0.002	2.67	1.00
	10% EtOH	0.002	330	2.25 (19%)	4.57 (81%)	4.13	0.007	2.41	0.98
	50% EtOH	0.009	330	2.98 (44%)	6.15 (55%)	4.75	0.040	2.06	0.99
	80% EtOH	0.014	330	3.22 (49%)	6.75 (51%)	5.00	0.050	1.94	1.00
	Only EtOH	0.017	330	3.38 (55%)	7.43 (45%)	5.18	0.055	1.87	1.04
3(Py$_2$ Am-^{Ar}TAA)	**MeOH**	0.004	330	1.8 (15%)	4.08 (85%)	3.74	0.013	2.66	0.94
	10% EtOH	0.012	330	2.12 (20%)	4.6 (80%)	4.10	0.029	2.40	0.95
	50%	0.025	330	3.23	6.21	4.62	0.05	2.11	1.00

	EtOH			(53%)	(46%)				
	80% EtOH	0.030	330	3.34 (54%)	6.8 (56%)	4.92	0.06	1.97	1.00
	Only EtOH	0.041	330	3.39 (56%)	7.1 (44%)	4.99	0.082	1.92	1.02
2 (PyAm-^{Ar}TAA)	**MeOH**	0.004	430	0.62 (30%)	4.35 (70%)	3.22	0.015	3.09	0.96
	10% EtOH	0.006	430	0.71 (16%)	4.36 (84%)	3.74	0.018	2.65	0.95
	50% EtOH	0.009	430	0.76 (19%)	4.72 (80%)	3.96	0.025	2.50	0.99
	80% EtOH	0.010	430	0.97 (27%)	5.04 (73%)	3.94	0.030	2.50	1.02
	Only EtOH	0.012	430	0.96 (29%)	5.25 (71%)	3.99	0.032	2.47	1.00
3 (Py_2Am-^{Ar}TAA)	**MeOH**	0.005	410	1.34 (33%)	6.74 (67%)	4.98	0.012	1.99	1.03
	10% EtOH	0.011	410	1.38 (32%)	7.14 (68%)	5.28	0.020	1.87	1.06
	50% EtOH	0.021	410	1.31 (29%)	7.32 (71%)	5.58	0.037	1.75	1.04
	80% EtOH	0.024	410	1.37 (25%)	7.94 (75%)	6.29	0.038	1.55	1.06
	Only EtOH	0.031	410	1.36 (22%)	8.03 (78%)	6.53	0.067	1.48	1.05
3 (Py_2Am-^{Ar}TAA)	**MeOH**	0.045	475	2.99 (53%)	12.56 (47%)	7.48	0.060	1.27	1.01
	10% EtOH	0.060	475	2.97 (54%)	12.73 (46%)	7.48	0.080	1.25	1.00
	50% EtOH	0.062	475	3.05 (54%)	12.74 (46%)	7.49	0.082	1.25	1.02
	80% EtOH	0.064	475	3.12 (47%)	12.93 (53%)	8.24	0.077	1.13	1.00
	Only EtOH	0.069	475	3.09 (52%)	13.30 (48%)	8.03	0.085	1.15	0.99
λ_{ex} = 375									
2 (PyAm-^{Ar}TAA)	**MeOH**	0.008	430	0.78 (34%)	4.51 (66 %)	3.24	0.024	3.06	0.98
	10% EtOH	0.010	430	1.17 (59%)	4.09 (40%)	2.34	0.042	4.23	0.98
	50% EtOH	0.015	430	1.39 (79%)	4.22 (21%)	1.98	0.075	4.97	0.96
	80% EtOH	0.022	430	1.4 (85%)	3.5 (15%)	1.71	0.122	5.72	0.93
	Only	0.028	430	1.43	3.75	1.69	0.213	5.70	0.97

	EtOH			(89%)	(11%)				
3 (Py_2Am-^{Ar}TAA)	**MeOH**	0.005	410	1.23 (26%)	6.69 (73%)	5.25	0.001	1.89	1.05
	10% EtOH	0.006	410	1.24 (34%)	6.64 (66%)	4.82	0.012	2.06	1.02
	50% EtOH	0.006	410	1.31 (52%)	6.61 (48%)	3.97	0.015	2.50	1.01
	80% EtOH	0.007	410	1.34 (60%)	6.14 (40%)	3.25	0.020	2.96	1.02
	Only EtOH	0.008	410	1.37 (63%)	6.04 (37%)	3.12	0.025	3.17	1.02
3 (Py_2Am-^{Ar}TAA)	**MeOH**	0.073	475	3.45 (50%)	15.87 (50%)	9.67	0.08	0.953	1.08
	10% EtOH	0.079	475	3.32 (49%)	15.70 (51%)	9.68	0.081	0.951	1.06
	50% EtOH	0.083	475	3.27 (49%)	15.51 (51%)	9.54	0.087	0.961	1.04
	80% EtOH	0.103	475	3.07 (49%)	14.81 (51%)	9.06	0.113	0.99	1.05
	Only EtOH	0.104	475	2.79 (48%)	13.74 (52%)	8.50	0.164	1.011	1.00
For lifetimes of the moleculesλ_{ex} = 290 nm for **1**, **2**, **3**and λ_{ex} = 375 for **2**,**3**.Concentration of the compound = 10 μM; $<\tau>$, k_f, and k_{nr} are weighted means from the biexponential fits: $<\tau> = 1/(\alpha_1/\tau_1 + \alpha_2/\tau_2)$, $k_f = \Phi_f/<\tau>$, and $k_{nr} = (1-\Phi_f)/<\tau>$.									

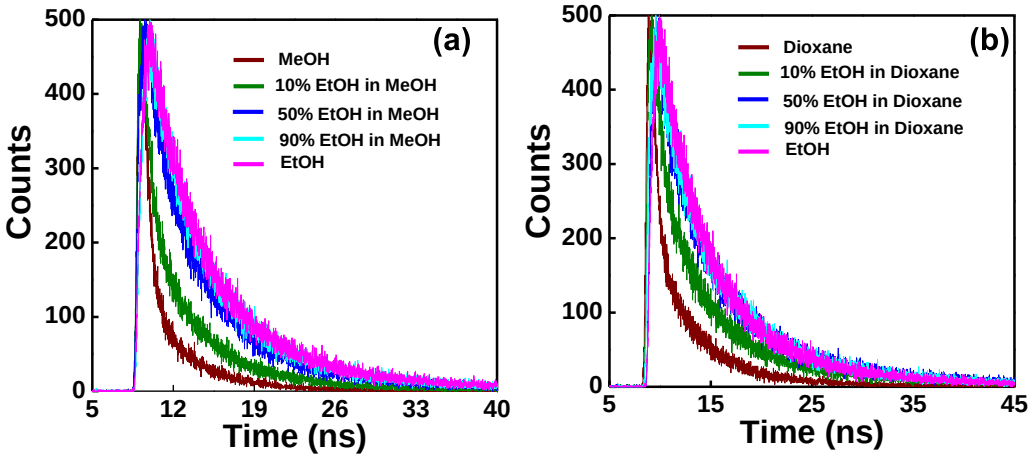


Figure S9. Time resolved fluorescence spectra of **1,** ^{Ar}**TAA**using 290 LED in (a) Methanol with increasing ethanol conc. (λ_{em} = 330 nm); (b) Dioxane with increasing ethanol conc. (λ_{em} = 330 nm).

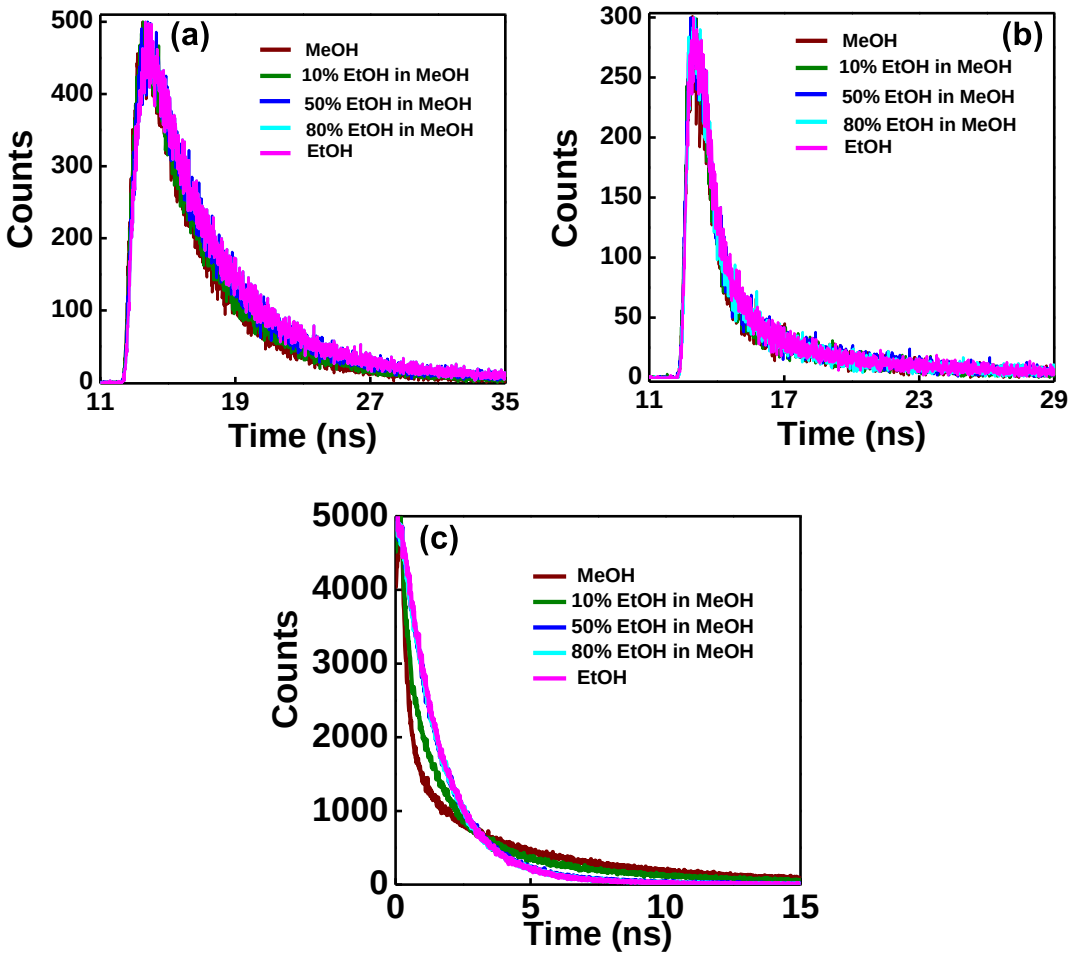


Figure S10. Time resolved fluorescence spectra of **2 (PyAm-^{Ar}TAA)**using 290 LED in methanol with increasing ethanol conc. (a) λ_{em} = 330 nm, (b) λ_{em} = 430 nm,(c) λ_{ex} = 375 nm, λ_{em} = 430 nm).

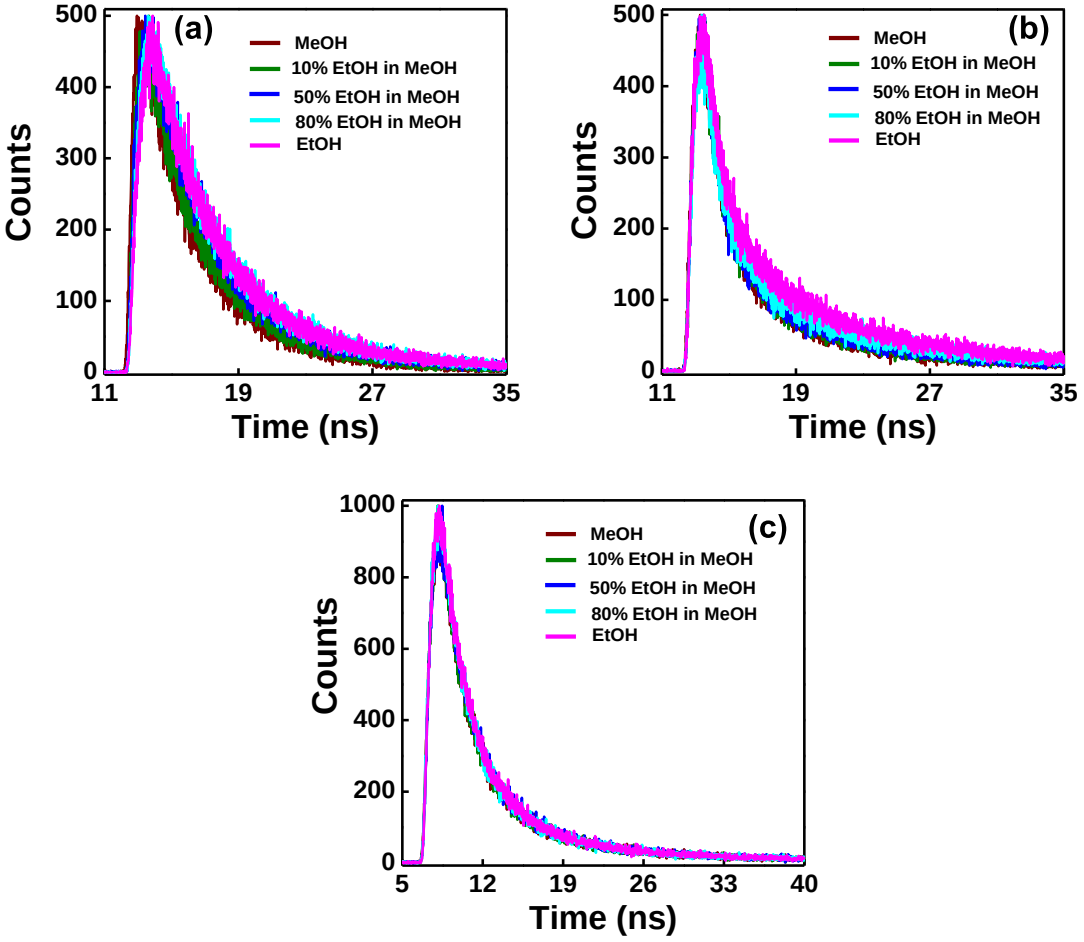


Figure S11. Time resolved fluorescence spectra of **3 (Py_2Am-^{Ar}TAA)**using 290 LED in in methanol with increasing ethanol conc. (a) λ_{em} = 330 nm, (b) λ_{em} = 410 nm and (c) λ_{em} = 460 nm.

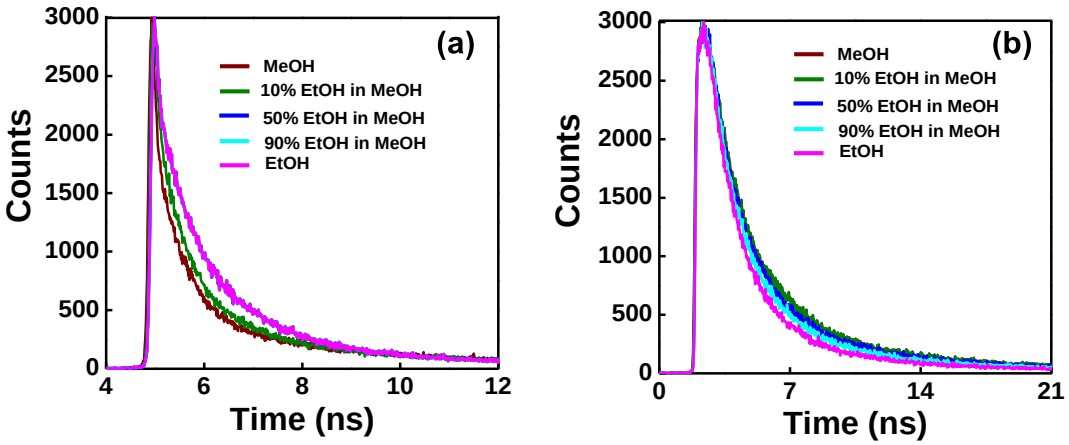


Figure S12. Time resolved fluorescence spectra of **3 (Py_2Am-^{Ar}TAA)**using 375 Laser inmethanol with increasing ethanol conc. (a) λ_{em} = 410 nm and (b) λ_{em} = 460 nm.

7. Picture of 1 (^{Ar}TAA), 2 (PyAm-^{Ar}TAA) and3 (Py_2Am-^{Ar}TAA) under Fluorescence light in MeOH and with increasing volume of EtOH solvent.

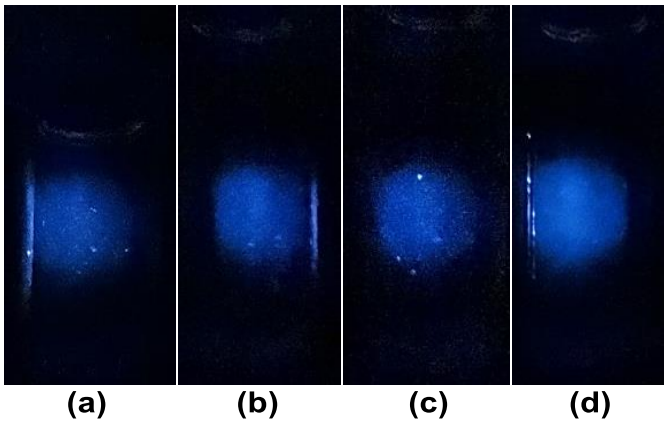


Figure S13. Picture under fluorescence light (λ_{ex} = 280 nm) of^{Ar}**TAA,1**in**(a)** MeOH **(b)** 10% EtOH in MeOH **(c)** 50% EtOH in MeOH (d) EtOHsolvents.

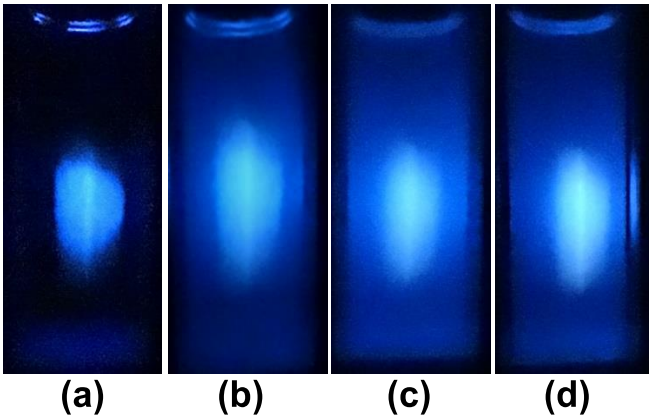


Figure S14. Picture under fluorescence light (λ_{ex} = 280 nm) of **PyAm-^{Ar}TAA,2**in **(a)** MeOH **(b)** 10% EtOH in MeOH **(c)** 50% EtOH in MeOH (d) EtOHsolvents.

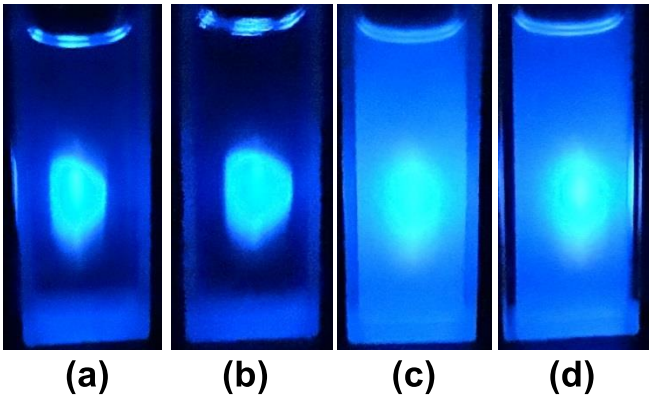


Figure S15. Picture under fluorescence light (λ_{ex} = 350 nm) of **PyAm-^{Ar}TAA,2**in **(a)** MeOH **(b)** 10% EtOH in MeOH **(c)** 50% EtOH in MeOH (d) EtOHsolvents.

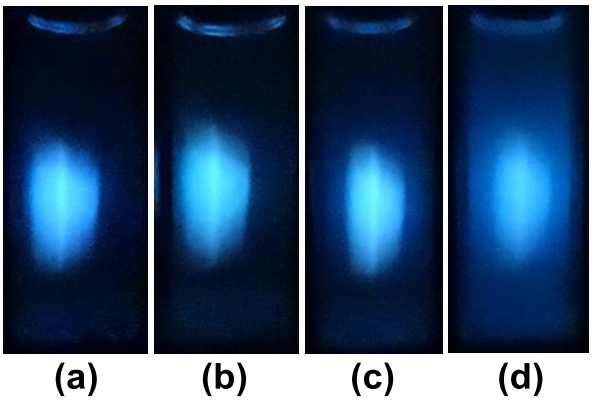


Figure S16. Picture under fluorescence light (λ_{ex} = 280 nm) of **3 (Py$_2$Am-^{Ar}TAA)**in **(a)** MeOH **(b)** 10% EtOH in MeOH **(c)** 50% EtOH in MeOH (d) EtOHsolvents.

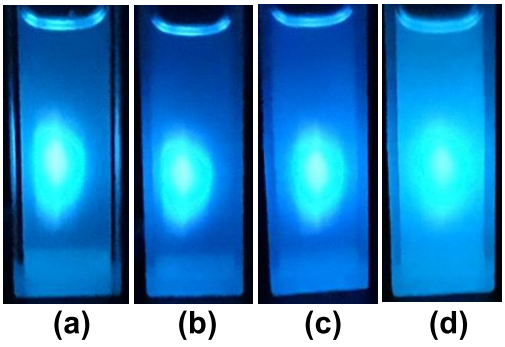


Figure S17. Picture under fluorescence light (λ_{ex} = 350 nm) of **3 (Py_2Am-^{Ar}TAA)**in **(a)** MeOH **(b)** 10% EtOH in MeOH **(c)** 50% EtOH in MeOH (d) EtOHsolvents.

Table S6. A comparative study table of other probes reported in the literature for Ethanol-MeOH detection.

Journal	Probe used	Observation	Detection limit
Present manuscript	Aromatic triazolo small molecular scaffold	Turn on fluorescence in Ethanol	0.243 (M)
Sens. Actuators B Chem. 2017, **245**, 406.	Triphenylamine-based fluorescent D-π-A system.	Strong fluorescence in methanol.	~ 0.7% (volume concentration)
ACS Appl. Mater. Interfaces 2015, **7**, 6189.	Terphenyl-ol (TPhOH) derivatives and sodium carbonate mixture.	Solid state sky blue fluorescence on exposed to ethanol vapour.	~ 5 v/v % ethanol
Mater. Lett. 2015, **159**, 5.	Flower-like SnO_2 aggregative nanosheets.	Selective gas diffusion to ethanol.	500 ppm ethanol at 300°C.
Anal. Chem. 2015, **87**, 4464	Ditrihexyl(tetradecyl)phosphonium bromothymol blue ($[P_{66614}]_2$[BTB]).	Colorimetric sensors of ethanol – methanol mixture.	---
ACS Appl. Mater. Interfaces 2013, **5**, 5927	A composite film prepared from oxoporphyrinogen (OxP) and a layered double hydroxide (LDH)	Color change magenta to purple in presence of methanol.	--
ACS Appl. Mater. Interfaces 2011, **3**, 4689	α-Fe_2O_3 hierarchical nanostructures.	Ethanol gas sensor.	100 ppm ethanol at 280°C.
Chem. Commun., 2010, **46**, 7022.	Comb-like Cu_2O nanorod.	Interface etching approach to detect ethanol.	---
J. Am. Chem. Soc. 2008, **130**, 3113	Hydroxyethyl methacrylate - polymerized crystalline colloidal array.	Sensitive sensor of ethanol.	---

8. Ethanol Vapor Sensing

For ethanol sensing purpose we have coated the glass plate by our compound through spin coating method. Then dry it and put on the mouth of glass vial containing methanol,

ethanol and mixture of both. After 5 minute interval of each sample we have measured the solid state fluorescence.

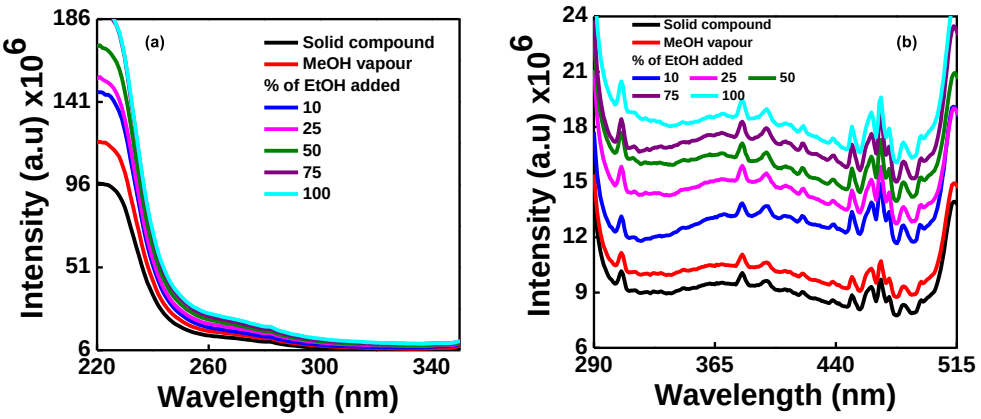


Figure S18. (a) Excitation (λ_{ex} = 390 nm) and fluorescence emission spectra (b) λ_{ex} = 280 nm of the **TriazolylAromatic Amino Acid Scaffold 1,** ^{Ar}**TAA**in presence of methanol vapour with increasing percentage of ethanol vapour (room temperature).

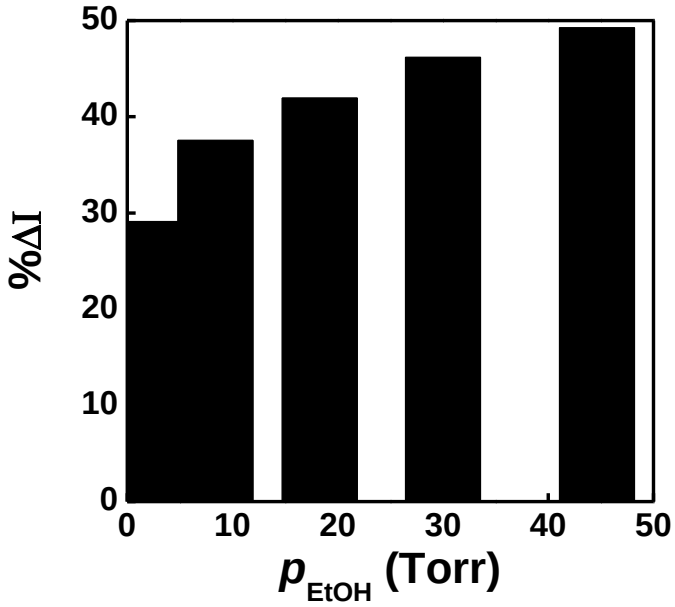


Figure S19. Plot of relative change of the fluorescence intensity, % ΔI with ethanol vapour pressure, P_{EtOH} (λ_{em} = 390 nm) of **1,** ^{Ar}**TAA**at room temperature.

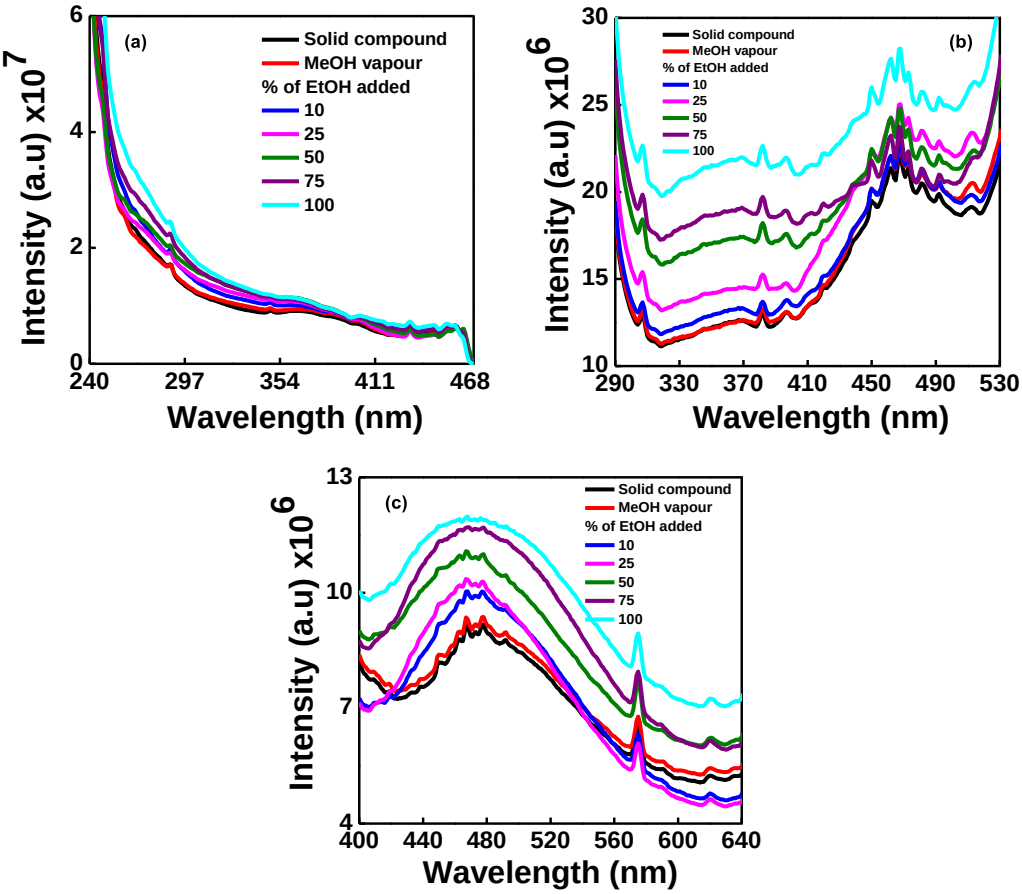


Figure S20. (a) Excitation (λ_{ex} = 480 nm), fluorescence emission spectra(b) λ_{ex} = 280 nm and (c) λ_{ex} = 350 nm **2 (PyAm-^{Ar}TAA)**in presence of methanol vapour with increasing percentage of ethanol vapour at room temperature.

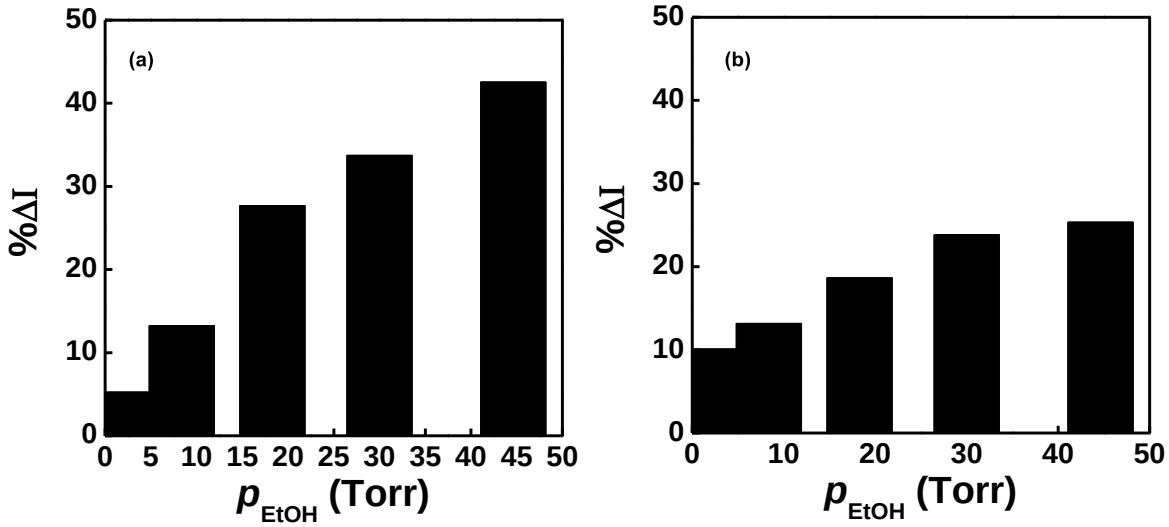


Figure S21. Plot of relative change of the fluorescence intensity, % ΔI with ethanol vapour pressure, P_{EtOH} (a) λ_{em} = 370 nm (b) λ_{em} = 470 nm of **2 (PyAm-^{Ar}TAA)** in presence of methanol vapour with increasing percentage of ethanol vapour at room temperature.

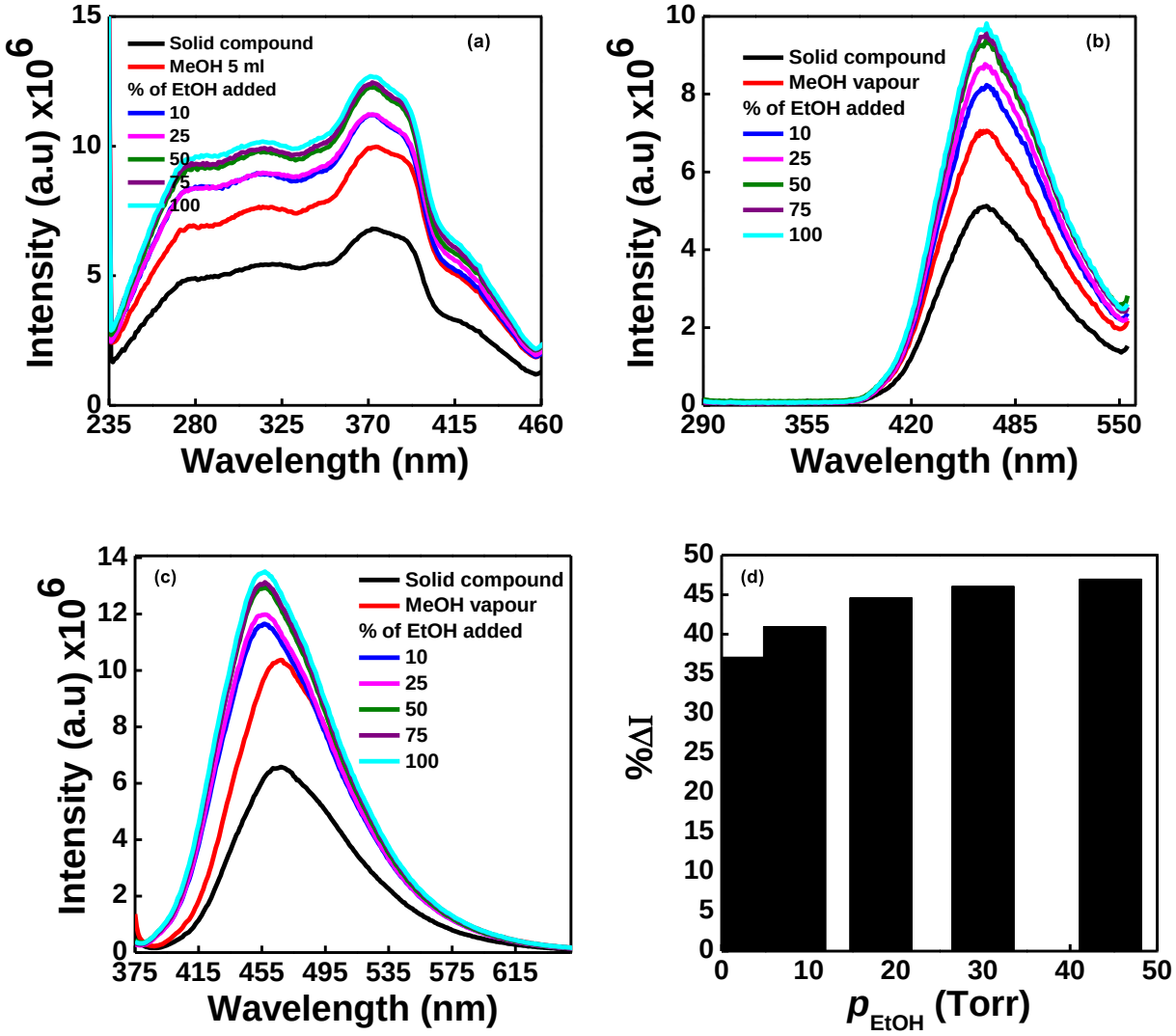


Figure S22. (a) Excitation (λ_{ex} = 470 nm), fluorescence emission spectra (b) λ_{ex} = 280 nm and (c) λ_{ex} = 370 nm (d) relative change of the fluorescence intensity, % ΔI with ethanol vapour pressure, P_{EtOH} (λ_{em} = 470 nm) of **3 (Py_2Am-^{Ar}TAA)**in presence of methanol vapour with increasing percentage of ethanol vapour at room temperature.

9. Determination of the Detection Limit

The limit of detection (LoD) has been calculated using the equation 3σ/K, where σ denotes the standard deviation of fluorescence intensity in MeOH solvent and K represents slope of plotting Intensity Vs concentration of added EtOH of methanol-ethanol titration experiment.

Table S7. Standard deviation and detection limit of ethanol sensing by our synthesized scaffold and pyrene derivative:

Repetition	Fluorescence Intensity		
	^{Ar}TAA	Py_1Amide_^{Ar}TAA	Py_2Amide_^{Ar}TAA
1	46911	29863	50845
2	47804	28919	44078
3	46795	31188	47744
4	50082	29099	47118
5	47083	32703	46408
6	49884	30220	50117
7	48355	29864	47808
8	48774	28864	49281
Average	48222	30090	47925
STDEV	1213	1225	2030
slope	14942.522	43440.63	53904.64
LoD	0.243 (M)	0.084 (M)	0.112 (M)

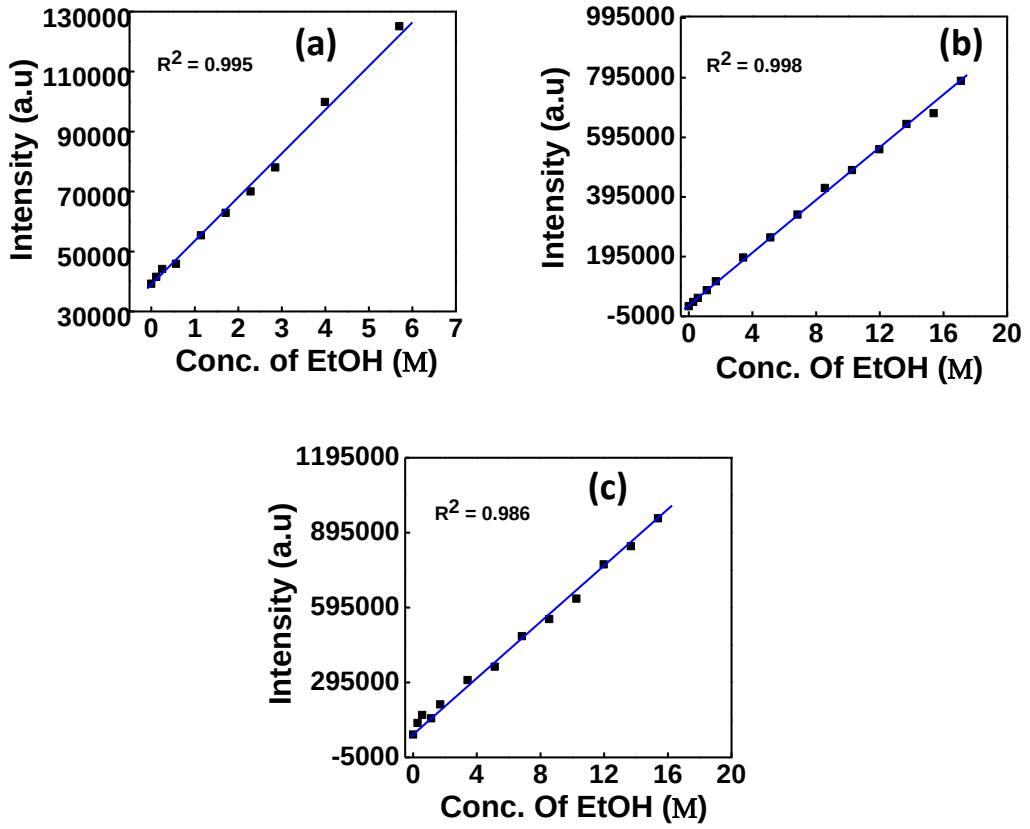


Figure S23. Plot of fluorescence intensity vs concentration of EtOH in MeOH of MeOH-EtOH titration for (a) **^{Ar}TAA** (**1**), (b) Py-Amide **^{Ar}TAA** (**2**), (c) **Py_2-Amide ^{Ar}TAA** (**3**).

10. Study of IR Spectroscopy

The differential H-bonding interaction was evident from IR spectra that showed the major differential perturbation and a noticeable change occurred at ester carbonyl and triazole-N=N stretching frequency, respectively. As a representative example, the ester carbonyl of scaffold **8** in solid KBr exhibited stretching frequency at 1719 cm^{-1} and triazole-N=N stretching appeared at 1441/1459 cm^{-1} while theamide Istretching was not observed. However, the sample when soaked with methanol, ethanol or a mixed solvent and recorded the IR we found nice differential stretching frequencies of all the above functional groups. Thus, while ester >C=O absorb at 1713 cm^{-1} along with the appearance of amide-I band at 1667 cm^{-1} in methanol, the scaffold behaved similar to the solid state in ethanol with a stretching frequency at 1716 cm^{-1} corresponding to ester>C=O. The triazole-N=N-stretching also in ethanol (1436/1458 cm^{-1}) was more correlating to a solid state compared to that observed in methanol (1418/1450 cm^{-1}). Soaking with a mixed ethanol:methanol (1:1) solvent, the ester >C=O stretching, triazole-N=N-stetching appeared at 1715 cm^{-1} and 1434/1452 cm^{-1}, respectively, along with appearance of amide-I at 1699 cm^{-1}. Similar observations were noted in case of scaffold. Therefore, it is clear that interactions such as H-bonding in methanol and ethanol are very much different and is more in methanol compared to ethanol.

Whereas, scaffold **1**exhibited acid carbonyl stretching frequency at 1702 $cm^{-1}$with amide-I band at 1687 cm^{-1} and triazole-N=N stretching appeared at 1440/1463 cm^{-1} in solid KBr. when the sample soaked with methanol acid>C=O absorb at 1699 $cm^{-1}$and amide-I band at 1668 cm^{-1}. Butwhenscaffold soaked in ethanol acid>C=O absorb at 1700 $cm^{-1}$with amide-I band at 1674 cm^{-1}. The triazole-N=N-stretching also in ethanol (1430/1454 cm^{-1}) was more correlating to a solid state compared to that observed in methanol (1406/1445 cm^{-1}).

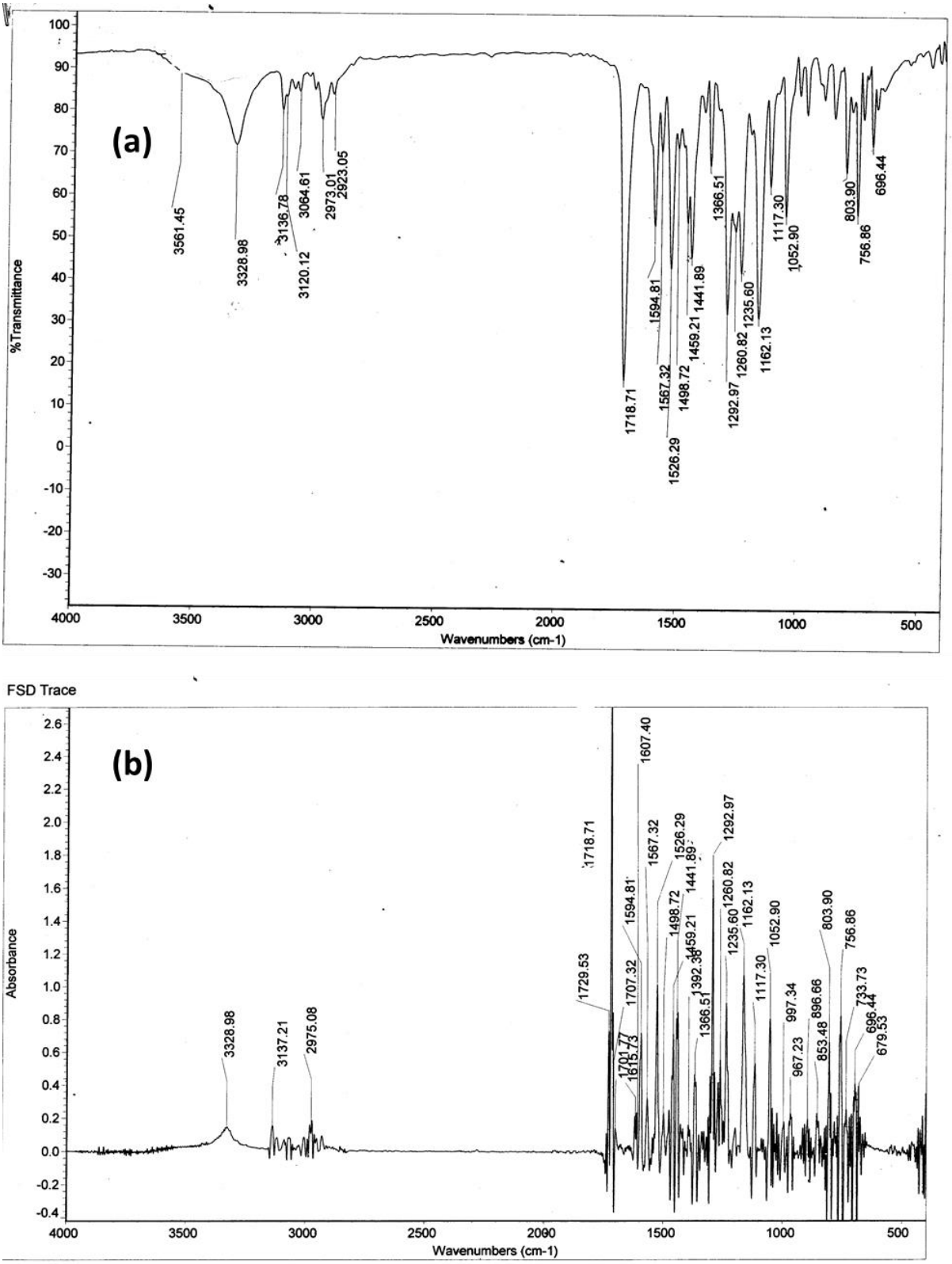


Figure S24. (a)IR spectra and (b) FSD traces of **8,** ^{Ar}**TAA**at dry and solid condition.

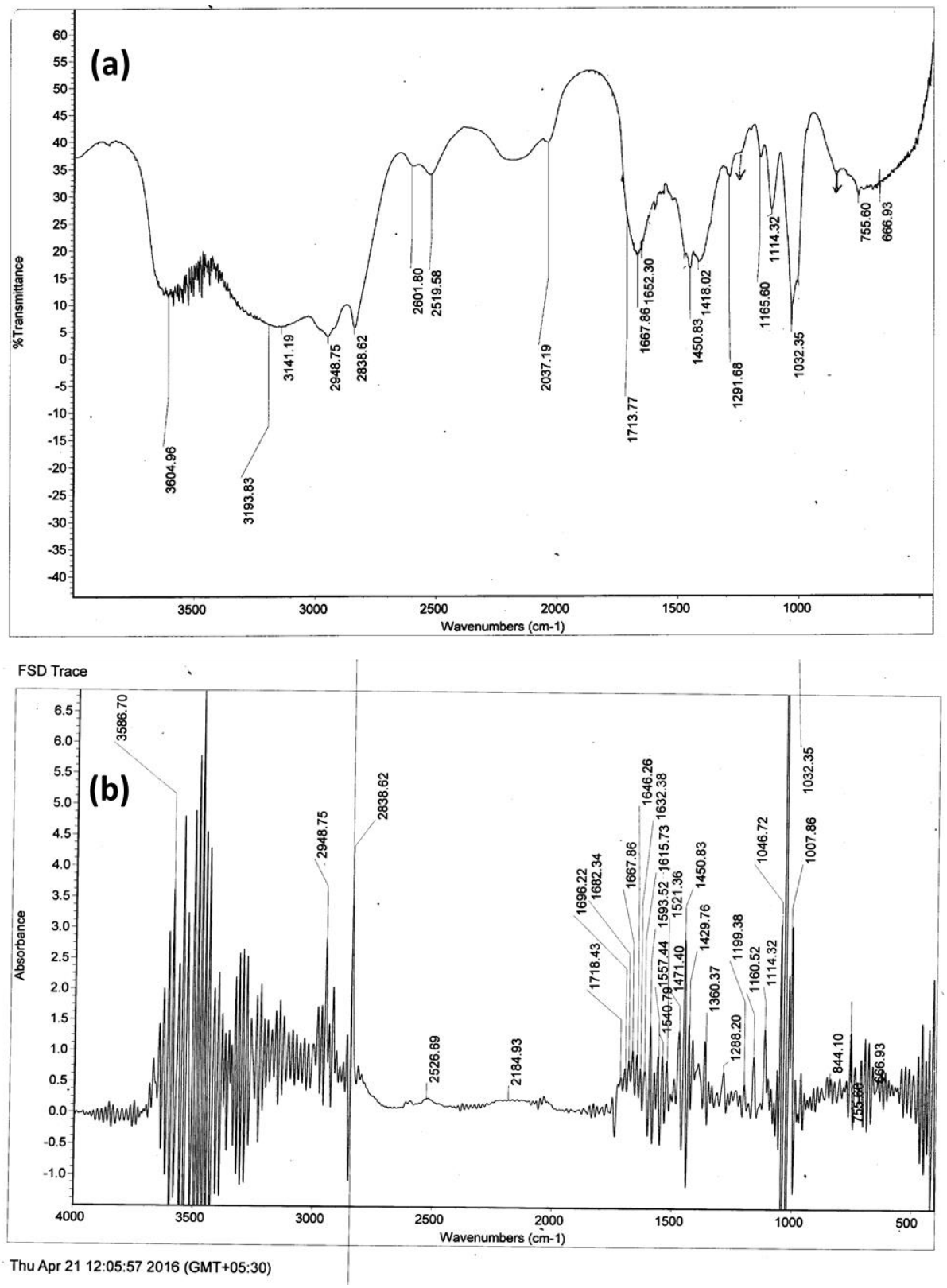


Figure S25. (a)IR spectra and (b) FSD traces of **8,** ^{Ar}**TAA**soakedin methanol.

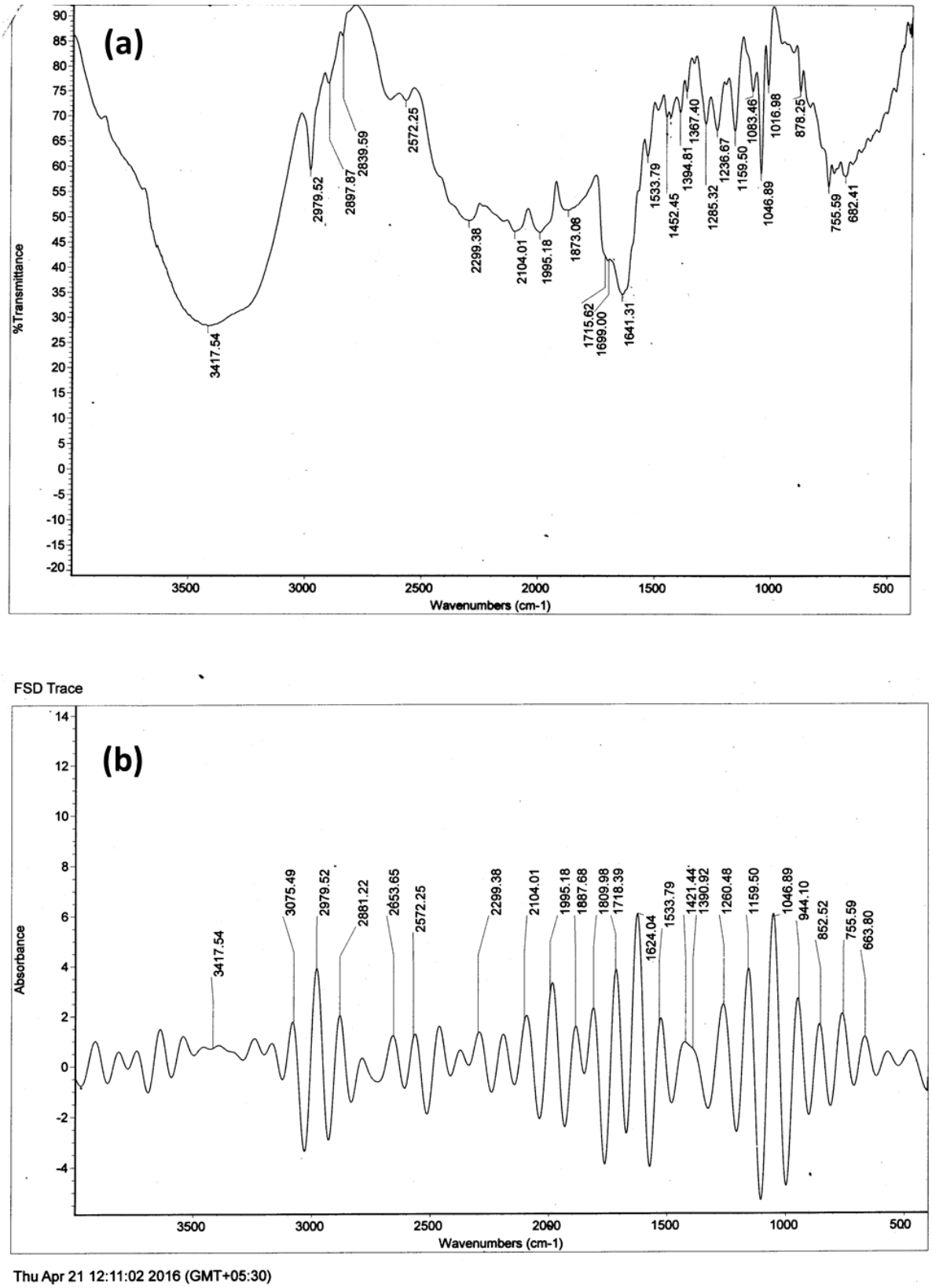


Figure S26. (a)IR spectra and (b) FSD traces of **8,** ^{Ar}**TAA**soakedin ethanol and methanol (1:1) mixture.

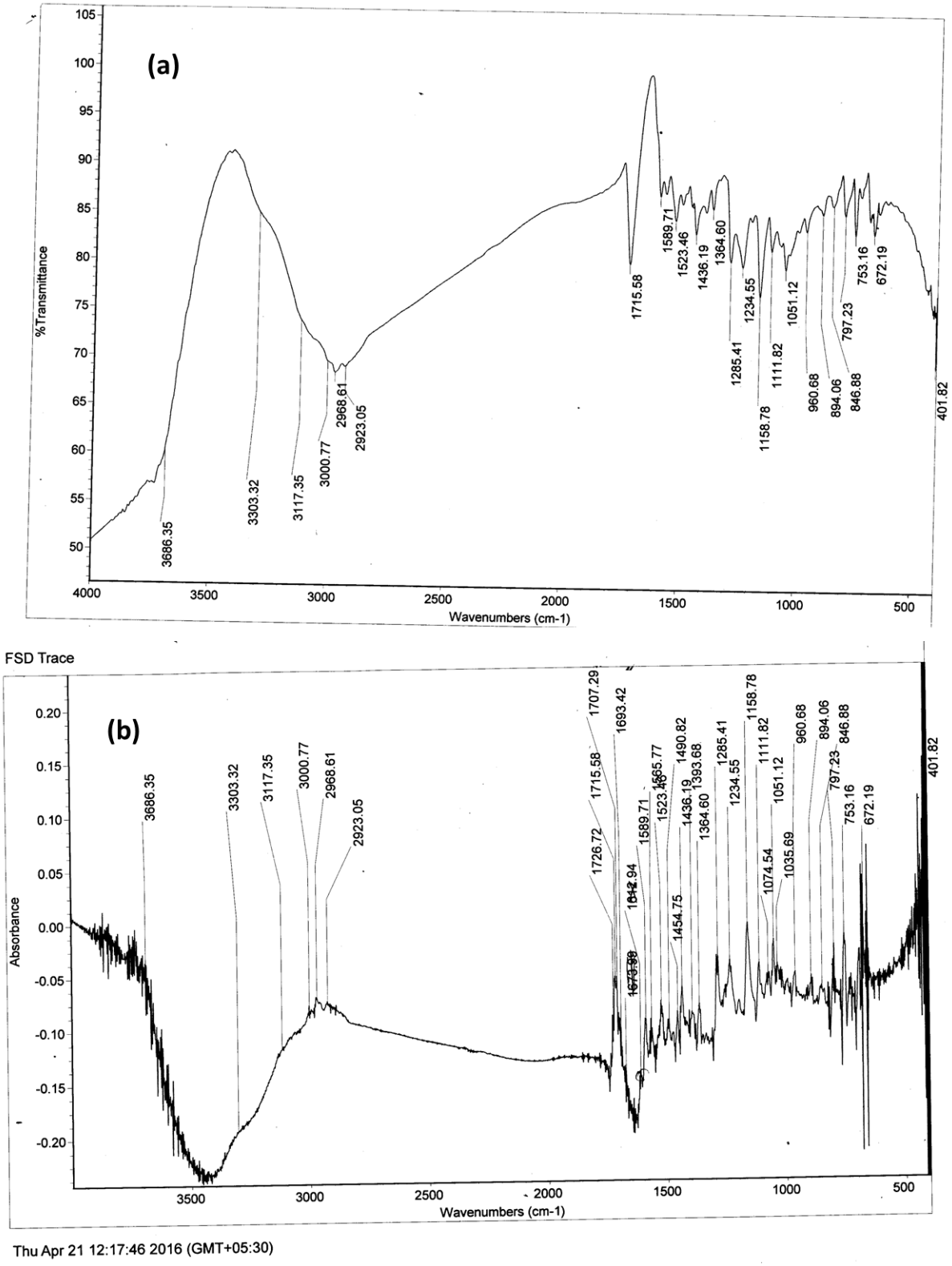


Figure S27. (a)IR spectra and (b) FSD traces of **8, ^{Ar}TAA**soakedin ethanol**.**

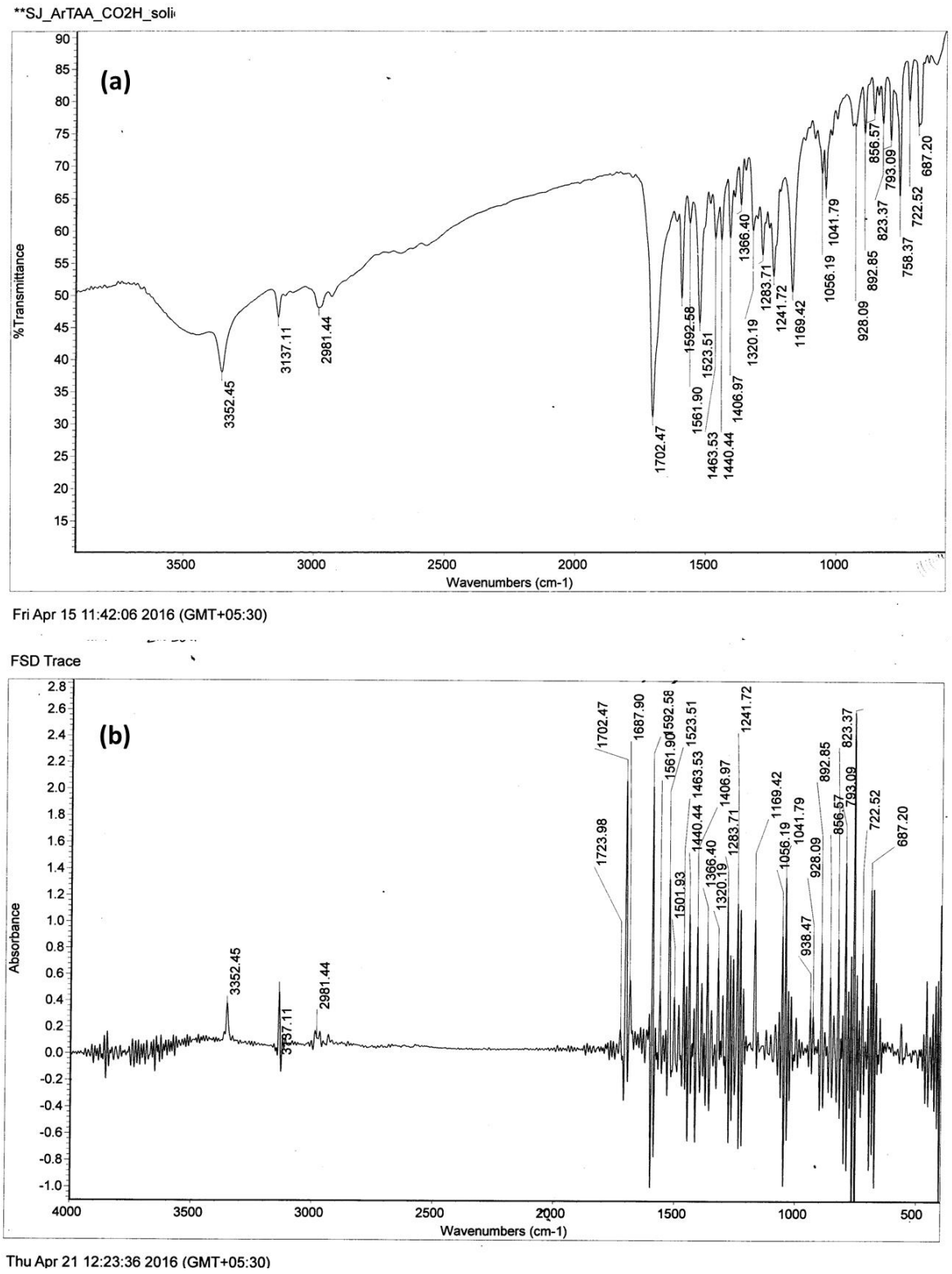


Figure S28. (a)IR spectra and (b) FSD traces of **1,** ^{Ar}**TAA**at dry and solid condition**.**

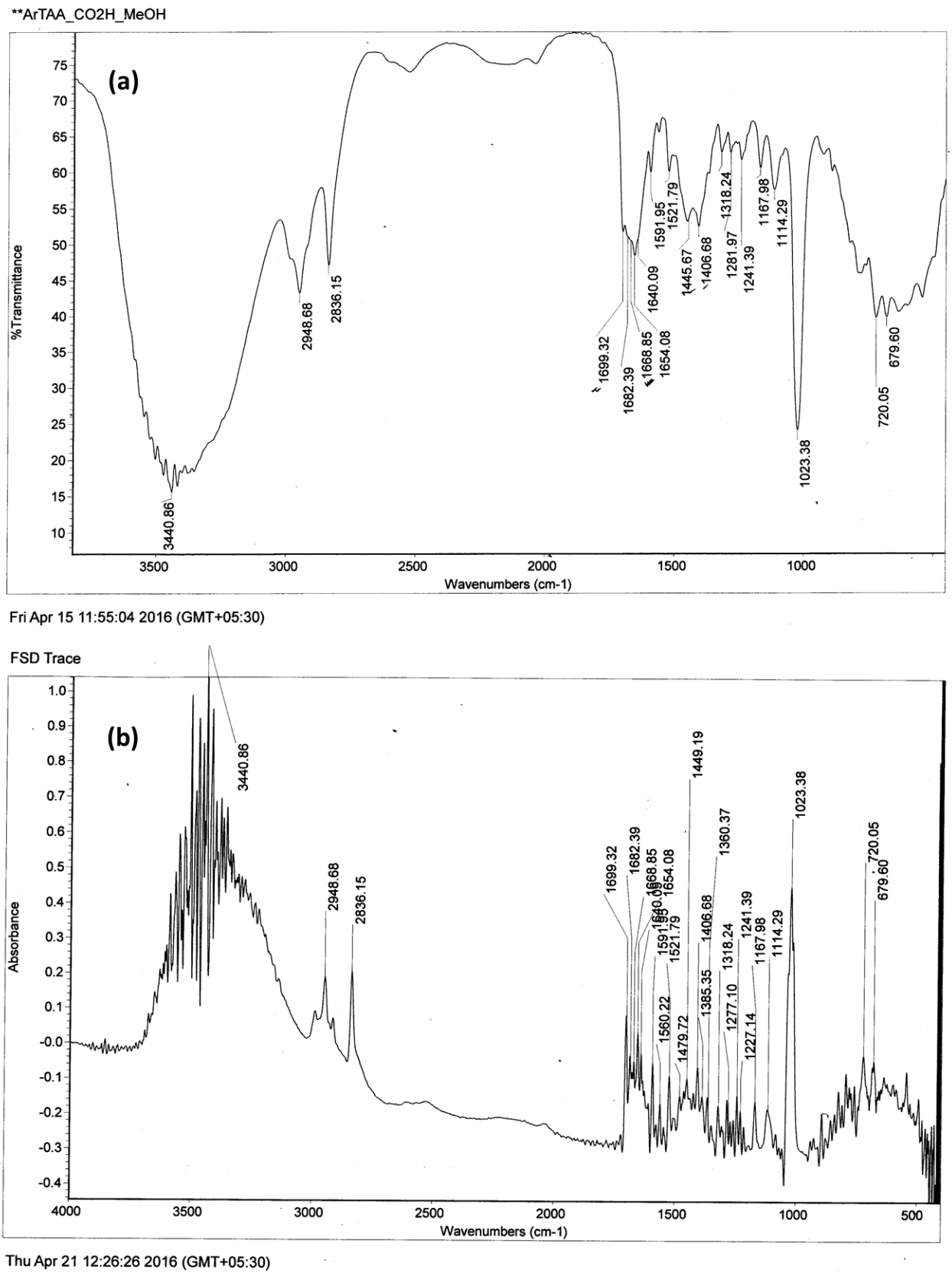
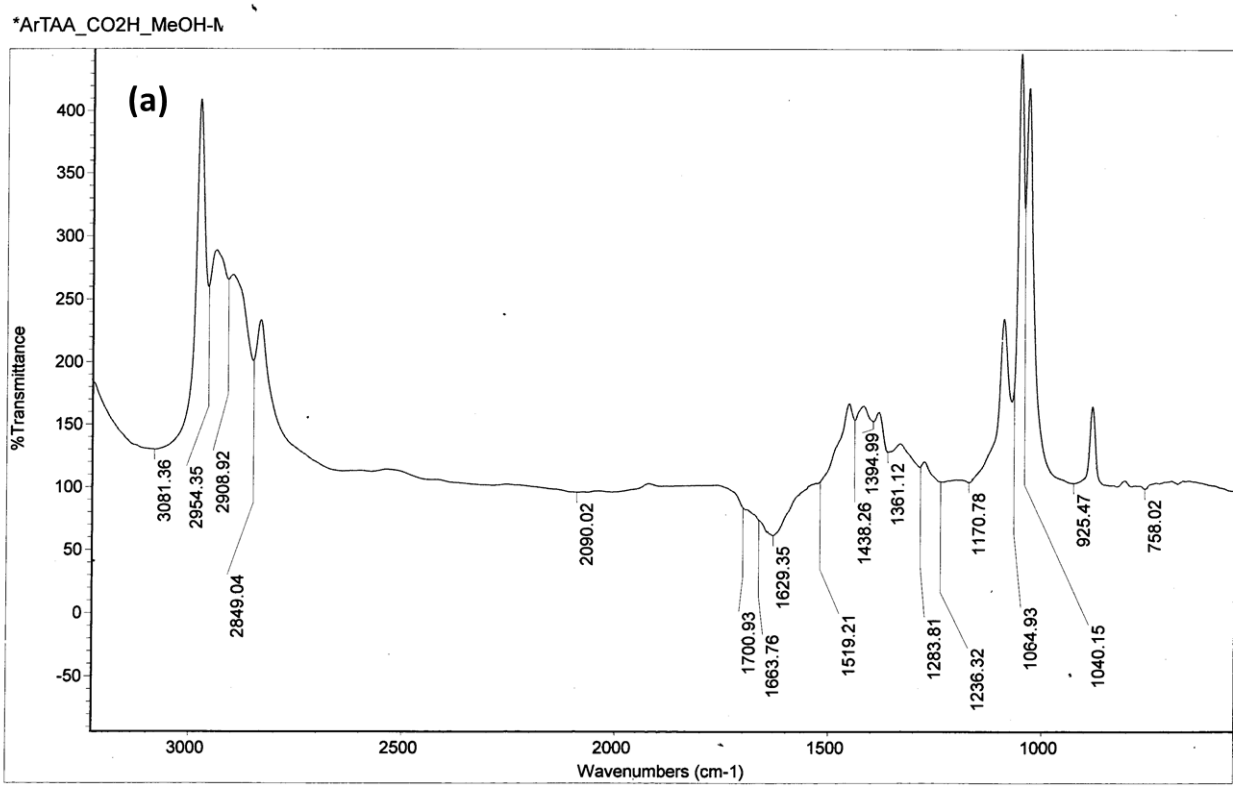


Figure S29. (a)IR spectra and (b) FSD traces of **1,** ^{Ar}**TAA**soaked in methanol.



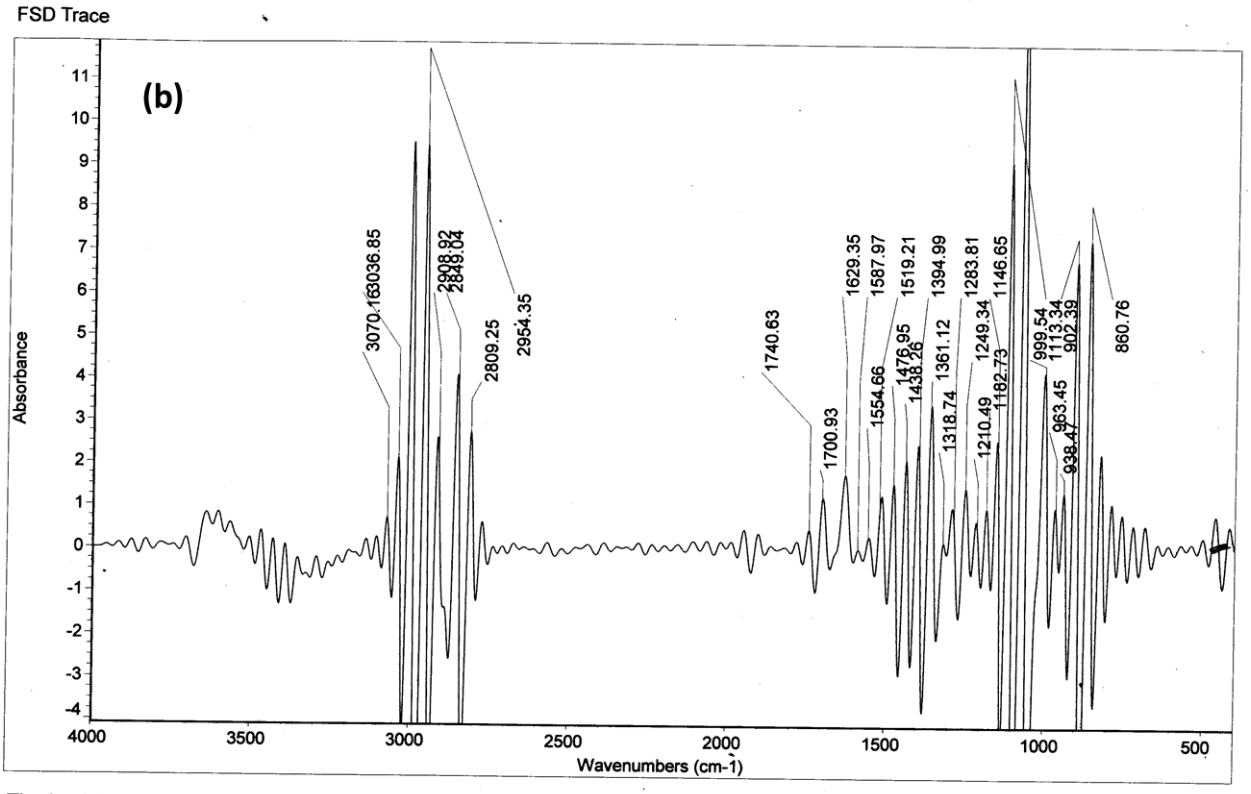


Figure S30. (a)IR spectra and (b) FSD traces of **1,** ^{Ar}**TAA**soaked in ethanol and methanol (1:1) mixture**.**

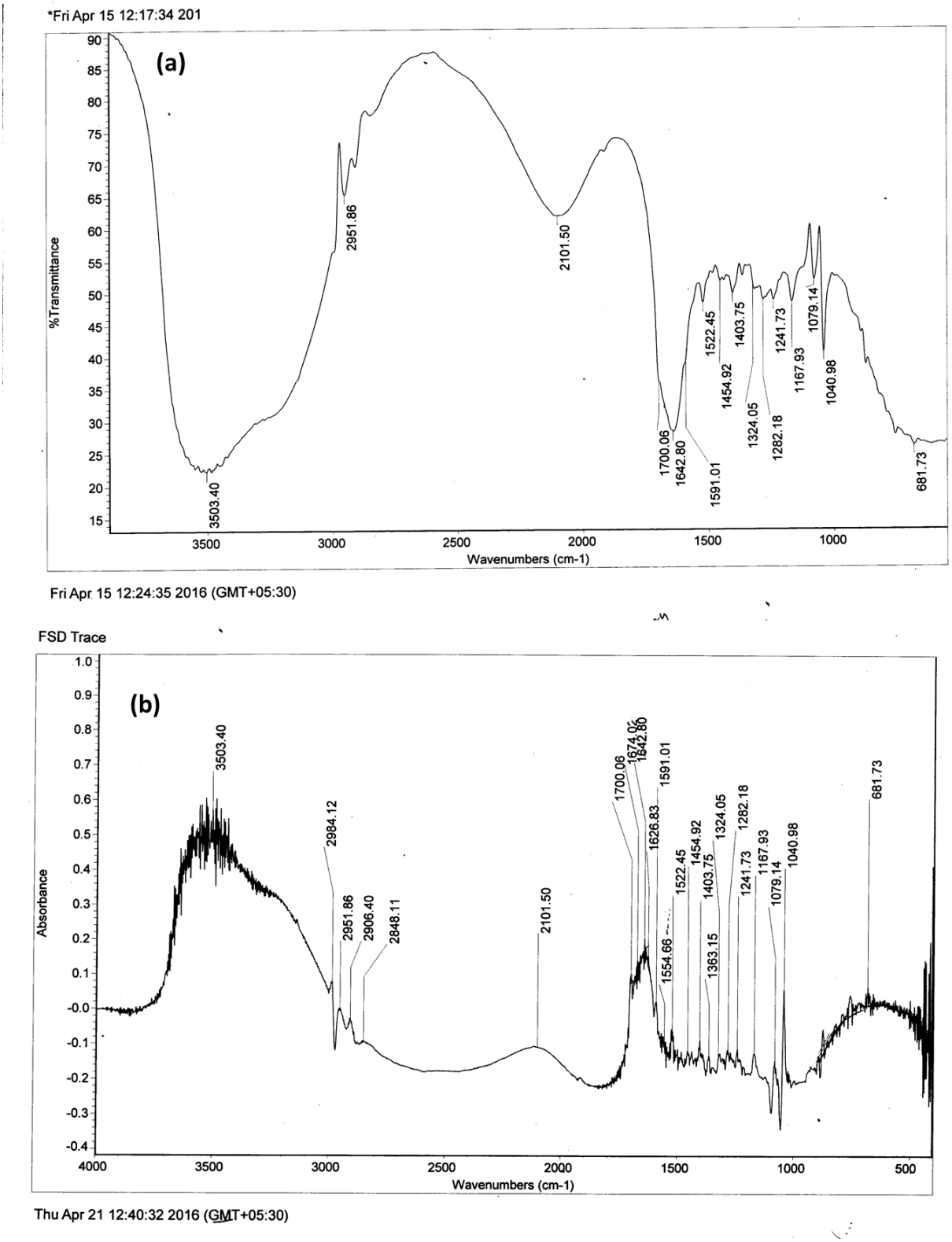


Figure S31. (a)IR spectra and (b) FSD traces of **1,** ^{Ar}**TAA**soaked in ethanol**.**

11.Study of Circular Dichroism Spectroscopy

Circular dichroism spectra were recorded using a CD spectropolarimeter with a cell path length of 10 mm at 25 ^{o}C. All the samples were prepared in spectroscopic grade solvent with 100 μM concentration.

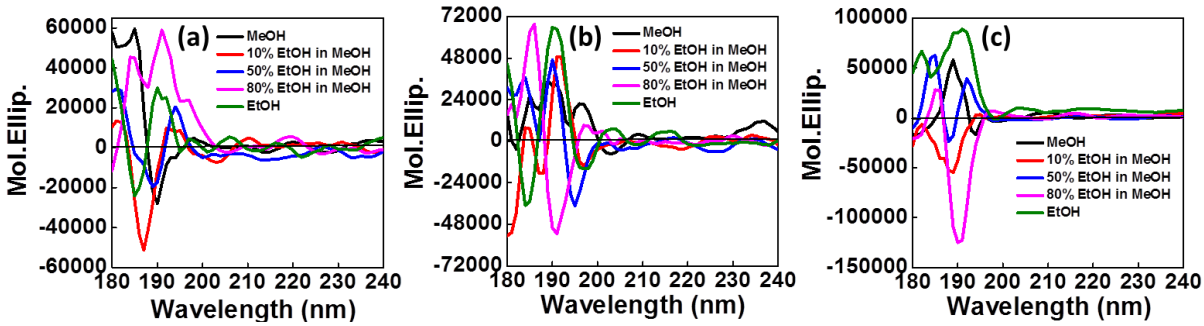


Figure S32. Deconvoluted molar ellipticity of synthesized amino acids scaffolds **1, ^{Ar}TAA (a);2 (PyAm-^{Ar}TAA) (b) and 3, Py$_2$Am-^{Ar}TAA (c)** in methanol and increasing volume of EtOH solvent (100 μM concentration).

12.Optimized Structure Using Maestro vs. 9.1

12.1. Optimization Structure of of Scaffold 8 with four MeOH/EtOH solvent molecule and Conformational Search of Optimized Structures

We are using Schrodinger Macromodel(Maestro vs. 9.1) software with Amber* force field in MeOH/EtOH (putiing their corresponding dielectric constant). A conjugate gradient minimization scheme [PRCG (Polak-Ribiere Conjugate Gradient)] that uses the Polak-Ribierefirst derivative method with restarts every 3N iterations was employed for the minimization ofthe peptides.

Next, we carried out conformational search using Amber* force field at respective dielectric in MeOH/EtOH with “large scale low-frequency-mode conformational search” (Mixed torsional/Large scale low-mode sampling = MCMM/LMCS) method.A total of 500 structures were processed with 500 maximum no. of steps iteration. A global search analysis eliminates redundant conformers using RMS deviation for all compared atoms exceed the threshold Cutoff of 0.5 Å. An optimal minimization method was chosen for minimizing the generating conformers.

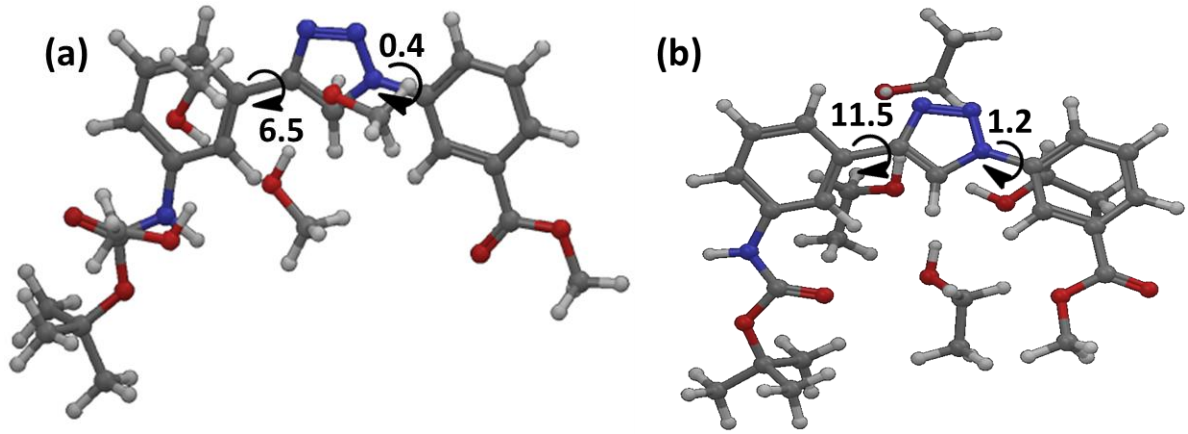


Figure S33. The conformer, obtained after conformational search, with 1.00 k.cal/mole (4.18 kJ/mole) global minimum. (a) **^{Ar}TAA** with four **MeOH** solvent molecule(b) scaffold **8**with four**EtOH**solvent molecule.

13. Optimized Structure Using Gaussian 09

The ground state structures of ^{Ar}TAA with four MeOH/EtOH solvent molecule and $Py_2{}^{Ar}$TAA were optimized using Gaussian 09 programme at B3LYP/6-31G level of theory with CPCM solvent model. The energy minimized geometry of the scaffold revealed that the aminophenyl unit remained almost in plane with triazole ring in both Methanol and ethanol solvent. However, the benzoic acid unit attained more out-of-planarity (33^o) in ethanol compared to that in methanol (20^o) with differential hydrogen bonding pattern. However, in case of **$Py_2{}^{Ar}$TAA**sensortwo pyrene moiety come closer in ethanol solvent compare to methanol where two fluorophoric unit are outward.

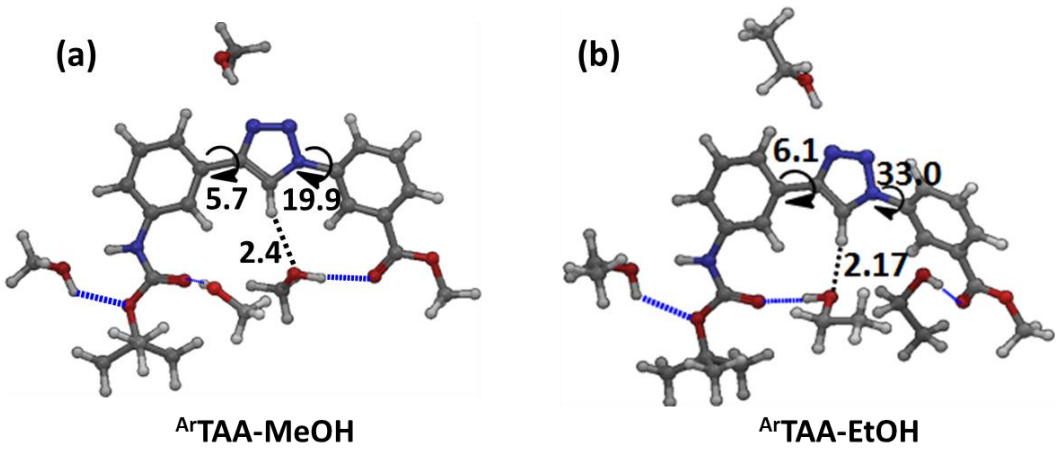


Figure S34.B3LYP/6-31G Optimized Structure of (a) **8**, **^{Ar}TAA-MeOH** in MeOH solvent (b) **8**, **^{Ar}TAA-EtOH** in EtOH solvent.

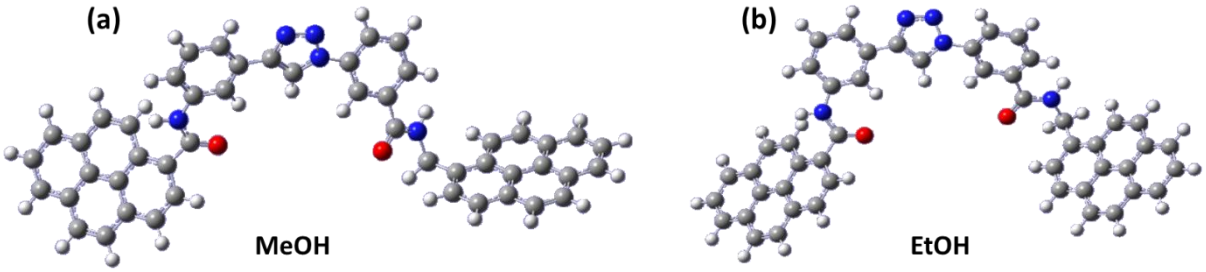
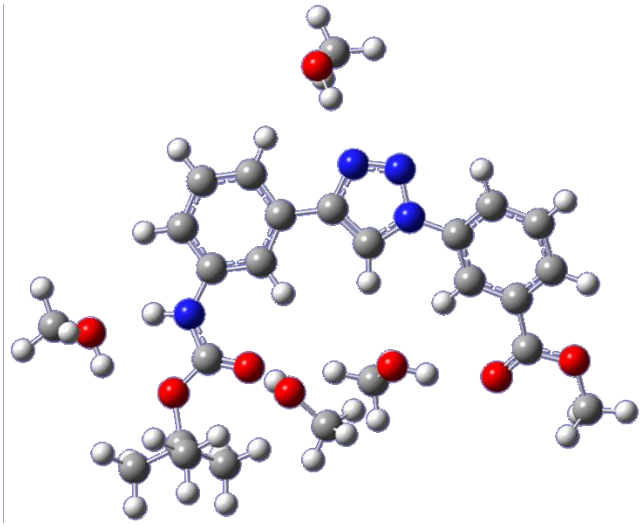


Figure S35.B3LYP/6-31G Optimized Structure of (a) **Py_2^{Ar}TAA** in MeOH solvent (b) **Py_2^{Ar}TAA** in EtOH solvent.

13.1. Cartesian Coordinates

B3LYP/6-31G Energy Optimized geometry and energy of**8, ^{Ar}TAA-MeOH**complex in MeOH solvent.



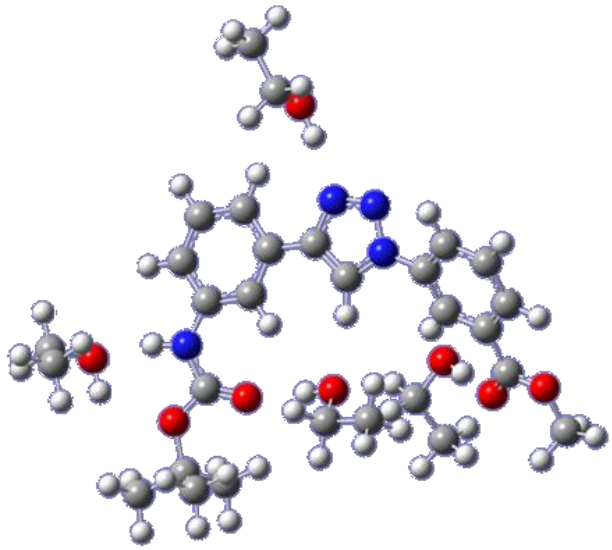
E(RB+HF-LYP)= -1796.20993340 a. u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.168432	-1.246187	-0.017561
2	6	0	4.063152	0.849193	0.434529
3	6	0	4.030201	-0.437911	-0.092424
4	1	0	3.132156	-0.822801	-0.557416
5	6	0	6.346548	-0.748518	0.555566

6	1	0	7.230177	-1.373457	0.608091
7	6	0	5.229428	1.354779	1.018278
8	1	0	5.238239	2.357421	1.428574
9	6	0	6.367682	0.550079	1.065035
10	1	0	7.275199	0.938729	1.515797
11	6	0	-0.591257	2.616036	0.040057
12	6	0	-1.444545	1.501353	-0.020149
13	1	0	-1.050779	0.499358	0.074611
14	6	0	-2.822204	1.677308	-0.199253
15	6	0	-1.120642	3.911061	-0.069624
16	1	0	-0.468897	4.776430	-0.015655
17	6	0	-2.493504	4.077081	-0.249251
18	1	0	-2.908131	5.077190	-0.338539
19	6	0	-3.343152	2.978025	-0.318063
20	1	0	-4.410993	3.118348	-0.461775
21	6	0	5.062114	-2.631656	-0.557257
22	6	0	6.216243	-4.629340	-1.070414
23	1	0	5.873597	-4.650799	-2.107107
24	1	0	5.558248	-5.244247	-0.452695
25	1	0	7.246376	-4.974962	-0.998498
26	6	0	-3.538518	-0.712468	-0.087160
27	6	0	-4.834728	-2.838319	-0.077188
28	6	0	-6.284964	-3.095843	-0.493874
29	1	0	-6.978135	-2.522059	0.130566
30	1	0	-6.520655	-4.158072	-0.376100
31	1	0	-6.443271	-2.823363	-1.542669
32	6	0	-4.634587	-3.164275	1.404879
33	1	0	-5.338987	-2.590928	2.017373
34	1	0	-3.619634	-2.948272	1.743469
35	1	0	-4.832702	-4.228985	1.569323
36	6	0	-3.873203	-3.597889	-0.995119
37	1	0	-4.105988	-4.667116	-0.948420
38	1	0	-2.833406	-3.453303	-0.700786
39	1	0	-3.997894	-3.269221	-2.032561
40	8	0	-4.703228	-1.373831	-0.283440
41	8	0	6.235351	-3.271454	-0.580496
42	8	0	4.017930	-3.145877	-0.941191
43	8	0	-2.465297	-1.235265	0.209196
44	6	0	0.856643	2.415292	0.202278
45	6	0	1.595845	1.246069	0.208760
46	1	0	1.323257	0.205287	0.108602
47	7	0	2.884549	1.648716	0.376479
48	7	0	-3.748494	0.620281	-0.285120
49	1	0	-4.717914	0.880675	-0.497973
50	7	0	2.957332	2.995213	0.470442
51	7	0	1.740508	3.452205	0.367528
52	8	0	1.310890	-2.153778	-0.672485
53	1	0	2.174100	-2.607576	-0.748292
54	8	0	-1.328358	-2.299723	2.595895
55	1	0	-1.695041	-1.876206	1.796567
56	8	0	-6.579027	0.840321	-0.848653

57	1	0	-6.477433	-0.127074	-0.834279
58	8	0	1.426623	6.327939	0.198545
59	1	0	1.578637	5.366217	0.330562
60	6	0	-7.401324	1.208776	0.263821
61	1	0	-7.475338	2.298506	0.256491
62	1	0	-8.409282	0.785803	0.171798
63	1	0	-6.965221	0.889972	1.219257
64	6	0	-0.581284	-3.431861	2.161913
65	1	0	-0.061870	-3.836096	3.036867
66	1	0	-1.227178	-4.225464	1.755178
67	1	0	0.164732	-3.167670	1.400790
68	6	0	0.595572	-2.352878	-1.890235
69	1	0	0.427226	-3.419002	-2.095031
70	1	0	-0.375393	-1.864975	-1.774637
71	1	0	1.113685	-1.907898	-2.750973
72	6	0	1.853188	6.638012	-1.120096
73	1	0	1.652969	7.700331	-1.292404
74	1	0	2.931193	6.467250	-1.262685
75	1	0	1.311197	6.060950	-1.884355

8, ^{Ar}TAA-EtOH complex in EtOH Solvent



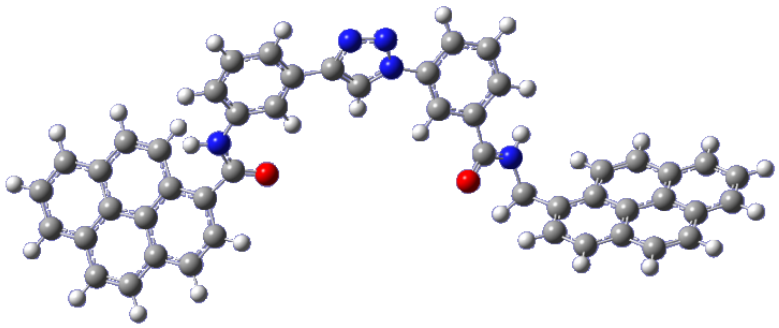
E(RB+HF-LYP)= -1953.48929795 a. u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.285885	-0.594697	0.485807
2	6	0	3.813063	1.311738	0.526899
3	6	0	4.066095	-0.001141	0.136336
4	1	0	3.343701	-0.554520	-0.453238

5	6	0	6.247307	0.136947	1.196781
6	1	0	7.190428	-0.326205	1.460781
7	6	0	4.766156	2.050803	1.235493
8	1	0	4.545107	3.069954	1.530308
9	6	0	5.985589	1.458049	1.557384
10	1	0	6.728851	2.027306	2.106202
11	6	0	-0.975296	2.334306	-0.438034
12	6	0	-1.686938	1.145762	-0.204161
13	1	0	-1.174257	0.270695	0.165973
14	6	0	-3.065626	1.090103	-0.437114
15	6	0	-1.652037	3.478644	-0.886886
16	1	0	-1.109935	4.400762	-1.068040
17	6	0	-3.029119	3.419734	-1.100729
18	1	0	-3.558444	4.302943	-1.447189
19	6	0	-3.736909	2.241511	-0.885571
20	1	0	-4.807560	2.202260	-1.066471
21	6	0	5.521259	-2.008771	0.077748
22	6	0	6.981353	-3.863852	0.192218
23	1	0	7.036746	-3.970803	-0.893150
24	1	0	6.217492	-4.535626	0.589556
25	6	0	-3.447531	-1.346999	-0.037088
26	6	0	-4.437181	-3.606536	0.238338
27	6	0	-5.904620	-4.041505	0.232211
28	1	0	-6.457942	-3.556700	1.043522
29	1	0	-5.971226	-5.124936	0.372196
30	1	0	-6.381328	-3.789212	-0.721081
31	6	0	-3.789432	-3.909730	1.591889
32	1	0	-4.329814	-3.399535	2.396460
33	1	0	-2.744054	-3.597793	1.613552
34	1	0	-3.835014	-4.987467	1.781593
35	6	0	-3.683463	-4.238710	-0.935038
36	1	0	-3.736220	-5.329504	-0.851215
37	1	0	-2.634316	-3.940063	-0.944369
38	1	0	-4.144685	-3.948294	-1.885099
39	8	0	-4.540869	-2.140381	0.046176
40	8	0	6.674506	-2.497789	0.544029
41	8	0	4.747517	-2.672672	-0.601954
42	8	0	-2.287052	-1.738747	0.047637
43	6	0	0.477254	2.361521	-0.210369
44	6	0	1.338354	1.327198	0.114848
45	1	0	1.174353	0.271985	0.301895
46	7	0	2.560929	1.912656	0.206607
47	7	0	-3.853766	-0.058477	-0.229659
48	1	0	-4.868644	0.067711	-0.310850
49	7	0	2.482042	3.240103	-0.047396
50	7	0	1.229654	3.505253	-0.296361
51	8	0	2.836962	-1.855738	-2.584180
52	1	0	3.513234	-2.165710	-1.951130
53	8	0	0.481743	-1.765462	0.597931
54	1	0	-0.443968	-1.777606	0.286679
55	8	0	-6.743306	-0.118763	-0.441712

56	1	0	-6.648955	-1.069855	-0.260408
57	8	0	0.525412	6.228126	-1.004975
58	1	0	0.831001	5.321691	-0.778080
59	6	0	-7.633049	0.438423	0.540530
60	1	0	-7.718010	1.497747	0.281365
61	1	0	-8.628987	-0.011495	0.429462
62	6	0	0.511662	-2.418555	1.871164
63	1	0	-0.126806	-1.885552	2.591252
64	1	0	0.118357	-3.441765	1.778765
65	6	0	1.788522	-2.827635	-2.587593
66	1	0	1.343664	-2.916923	-1.586532
67	1	0	1.013513	-2.428184	-3.252169
68	6	0	0.299052	6.920378	0.219615
69	1	0	-0.408355	6.367058	0.857680
70	1	0	1.236683	7.021042	0.790198
71	6	0	1.946268	-2.457169	2.370317
72	1	0	2.590989	-2.975790	1.652206
73	1	0	2.337295	-1.443667	2.511416
74	1	0	2.001150	-2.983375	3.329584
75	6	0	2.256824	-4.190637	-3.090281
76	1	0	3.030440	-4.603379	-2.431182
77	1	0	1.423391	-4.903011	-3.119721
78	1	0	2.676857	-4.107634	-4.099055
79	6	0	-7.125432	0.271781	1.967228
80	1	0	-7.824991	0.731416	2.674837
81	1	0	-7.030088	-0.788481	2.230585
82	1	0	-6.146721	0.747259	2.092708
83	1	0	7.948465	-4.067405	0.649463
84	6	0	-0.260731	8.299026	-0.095835
85	1	0	-1.210439	8.215555	-0.636169
86	1	0	-0.435552	8.865638	0.825483
87	1	0	0.439612	8.864207	-0.721157

3, (Py_2Am-^{Ar}TAA)in MeOH Solvent

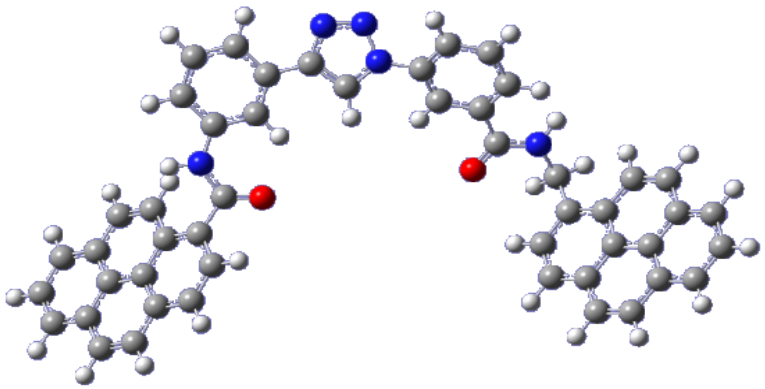


E(RB+HF-LYP)= -2310.1037 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.402505	1.647456	0.560972
2	6	0	-1.755463	3.410592	0.434451
3	6	0	-2.138379	2.098317	0.165048
4	1	0	-1.482597	1.414935	-0.362116
5	6	0	-4.288994	2.535439	1.184155
6	1	0	-5.292311	2.220875	1.453988
7	6	0	-2.631470	4.298068	1.069414
8	1	0	-2.315812	5.314788	1.270745
9	6	0	-3.901832	3.854338	1.428054
10	1	0	-4.593321	4.541043	1.905933
11	6	0	3.076030	3.923178	-0.732818
12	6	0	3.669980	2.653059	-0.660628
13	1	0	3.086417	1.778033	-0.413581
14	6	0	5.038637	2.502663	-0.918574
15	6	0	3.854705	5.041188	-1.067714
16	1	0	3.391470	6.019869	-1.122724
17	6	0	5.215185	4.883306	-1.326434
18	1	0	5.820363	5.747008	-1.586408
19	6	0	5.811138	3.627853	-1.253831
20	1	0	6.873017	3.514301	-1.456673
21	6	0	-3.749128	0.217526	0.236692
22	6	0	-5.152932	-1.738073	0.805866
23	1	0	-4.341579	-2.266242	0.302143
24	1	0	-5.293921	-2.206408	1.783059
25	6	0	5.203321	0.008277	-0.611877
26	8	0	-3.186588	-0.379172	-0.687302
27	8	0	4.004776	-0.224103	-0.448712
28	6	0	1.641587	4.085540	-0.457854
29	6	0	0.696757	3.158838	-0.054970
30	1	0	0.756839	2.108917	0.180984
31	7	0	-0.459413	3.863609	0.054524
32	7	0	5.709504	1.262641	-0.853844
33	1	0	6.698239	1.304543	-1.067111
34	7	0	-0.250404	5.168129	-0.265678
35	7	0	1.008408	5.297477	-0.570290
36	6	0	6.217385	-1.104019	-0.634924
37	6	0	5.861949	-2.226811	-1.395431
38	6	0	7.451238	-1.083297	0.064267
39	6	0	6.723409	-3.304893	-1.541171
40	1	0	4.896957	-2.231526	-1.892054
41	6	0	8.341250	-2.198667	-0.084330
42	6	0	7.845650	-0.023692	0.959233
43	6	0	7.976148	-3.309629	-0.906287
44	1	0	6.434291	-4.152950	-2.155930
45	6	0	9.600873	-2.210449	0.591201
46	6	0	9.043988	-0.043773	1.607244
47	1	0	7.162841	0.798952	1.139008

48	6	0	8.895325	-4.404468	-1.052737
49	6	0	10.497045	-3.312115	0.424971
50	6	0	9.973105	-1.123621	1.438656
51	1	0	9.310225	0.767591	2.279775
52	6	0	10.101310	-4.404476	-0.420382
53	1	0	8.603751	-5.239234	-1.684676
54	6	0	11.733461	-3.295638	1.092108
55	6	0	11.217912	-1.151450	2.089442
56	1	0	10.787016	-5.239010	-0.542312
57	6	0	12.088212	-2.226241	1.913876
58	1	0	12.415148	-4.132031	0.961126
59	1	0	11.496052	-0.322623	2.735252
60	1	0	13.047981	-2.232251	2.422522
61	6	0	-6.410898	-1.821399	-0.042799
62	6	0	-7.705182	-1.659703	0.508737
63	6	0	-6.273478	-2.046463	-1.417312
64	6	0	-8.847024	-1.737181	-0.354050
65	6	0	-7.937927	-1.418448	1.910002
66	6	0	-7.377103	-2.121443	-2.261381
67	1	0	-5.274740	-2.159462	-1.829842
68	6	0	-10.165269	-1.581213	0.176400
69	6	0	-8.676275	-1.971479	-1.753892
70	6	0	-9.194984	-1.268410	2.413968
71	1	0	-7.092919	-1.355099	2.587596
72	1	0	-7.237742	-2.300289	-3.324478
73	6	0	-10.354905	-1.343242	1.571799
74	6	0	-11.303218	-1.661197	-0.686260
75	6	0	-9.838670	-2.047178	-2.597076
76	1	0	-9.338257	-1.087988	3.476387
77	6	0	-11.658781	-1.192626	2.073794
78	6	0	-12.588007	-1.504717	-0.139984
79	6	0	-11.092970	-1.899611	-2.088497
80	1	0	-9.692173	-2.226644	-3.659205
81	6	0	-12.761323	-1.273380	1.224601
82	1	0	-11.799469	-1.011947	3.136442
83	1	0	-13.452300	-1.565854	-0.796432
84	1	0	-11.962196	-1.959516	-2.738591
85	1	0	-13.762966	-1.154916	1.628281
86	7	0	-4.686026	-0.367139	1.027170
87	1	0	-5.061585	0.146521	1.811398

3, (Py_2Am-^{Ar}TAA)in EtOH Solvent



E(RB+HF-LYP)= -2310.1045 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.685772	2.591249	0.672768
2	6	0	-2.003187	4.136247	-0.117603
3	6	0	-2.341398	2.955940	0.540758
4	1	0	-1.583507	2.309751	0.968170
5	6	0	-4.680644	3.417663	0.133549
6	1	0	-5.727918	3.136736	0.185533
7	6	0	-2.992795	4.969990	-0.649512
8	1	0	-2.710930	5.880133	-1.165422
9	6	0	-4.329580	4.601782	-0.517195
10	1	0	-5.102837	5.234495	-0.941272
11	6	0	2.962882	4.288326	-0.624573
12	6	0	3.424304	2.962613	-0.613907
13	1	0	2.741025	2.135546	-0.488331
14	6	0	4.789634	2.692186	-0.769918
15	6	0	3.872436	5.343771	-0.787831
16	1	0	3.511443	6.366157	-0.796749
17	6	0	5.230436	5.067388	-0.939857
18	1	0	5.937335	5.882349	-1.066273
19	6	0	5.694481	3.755326	-0.932847
20	1	0	6.755423	3.550265	-1.051905
21	6	0	-3.966574	1.295263	1.388792
22	6	0	-5.605413	-0.074313	2.624366
23	1	0	-4.743410	-0.405804	3.208143
24	1	0	-6.391615	0.206329	3.329566
25	6	0	4.683219	0.180146	-0.634401
26	8	0	-3.091980	0.430627	1.503353
27	8	0	3.462714	0.069065	-0.509598
28	6	0	1.528532	4.568423	-0.472319

29	6	0	0.458251	3.699809	-0.356306
30	1	0	0.385261	2.624566	-0.366690
31	7	0	-0.633319	4.501725	-0.256548
32	7	0	5.326317	1.386603	-0.773997
33	1	0	6.320752	1.337766	-0.956256
34	7	0	-0.265824	5.809726	-0.305427
35	7	0	1.029070	5.845584	-0.436079
36	6	0	5.567810	-1.034312	-0.727035
37	6	0	5.087750	-2.058869	-1.555261
38	6	0	6.795568	-1.199347	-0.035679
39	6	0	5.819679	-3.216799	-1.774477
40	1	0	4.129096	-1.921351	-2.044853
41	6	0	7.552691	-2.396958	-0.261936
42	6	0	7.308123	-0.252752	0.923800
43	6	0	7.063343	-3.404637	-1.149821
44	1	0	5.435659	-3.985526	-2.439531
45	6	0	8.803220	-2.595602	0.401550
46	6	0	8.497125	-0.450659	1.559319
47	1	0	6.722810	0.627572	1.164020
48	6	0	7.850828	-4.585695	-1.372086
49	6	0	9.567686	-3.779143	0.158379
50	6	0	9.297711	-1.615078	1.313562
51	1	0	8.853750	0.279471	2.281316
52	6	0	9.049397	-4.763549	-0.750797
53	1	0	7.464879	-5.339674	-2.053075
54	6	0	10.798704	-3.945877	0.814727
55	6	0	10.532074	-1.825628	1.950808
56	1	0	9.635336	-5.661331	-0.930219
57	6	0	11.274146	-2.978654	1.699670
58	1	0	11.380707	-4.844132	0.625356
59	1	0	10.903386	-1.076987	2.645806
60	1	0	12.227674	-3.126317	2.198591
61	7	0	-5.212552	1.141658	1.906541
62	1	0	-5.856930	1.918427	1.889076
63	6	0	-6.055107	-1.208654	1.717371
64	6	0	-7.335663	-1.223534	1.112447
65	6	0	-5.170010	-2.264027	1.474072
66	6	0	-7.695417	-2.319740	0.263094
67	6	0	-8.308821	-0.180269	1.310781
68	6	0	-5.512665	-3.333682	0.652089
69	1	0	-4.187056	-2.236773	1.934995
70	6	0	-8.981158	-2.358843	-0.360457
71	6	0	-6.769992	-3.384992	0.033063
72	6	0	-9.534391	-0.218620	0.716233
73	1	0	-8.064456	0.659756	1.952304
74	1	0	-4.802522	-4.139194	0.483392
75	6	0	-9.918270	-1.303572	-0.141631
76	6	0	-9.337651	-3.454123	-1.208228
77	6	0	-7.156275	-4.473616	-0.823536
78	1	0	-10.248265	0.583380	0.886775
79	6	0	-11.176767	-1.360050	-0.764715

80	6	0	-10.606880	-3.468211	-1.809982
81	6	0	-8.381266	-4.507529	-1.416599
82	1	0	-6.441742	-5.276105	-0.988841
83	6	0	-11.514387	-2.432021	-1.589281
84	1	0	-11.887739	-0.555293	-0.595721
85	1	0	-10.876918	-4.301106	-2.454282
86	1	0	-8.658785	-5.337268	-2.061827
87	1	0	-12.491310	-2.461047	-2.063693

14. ^{1}H and ^{13}C NMR spectra of synthesized compound

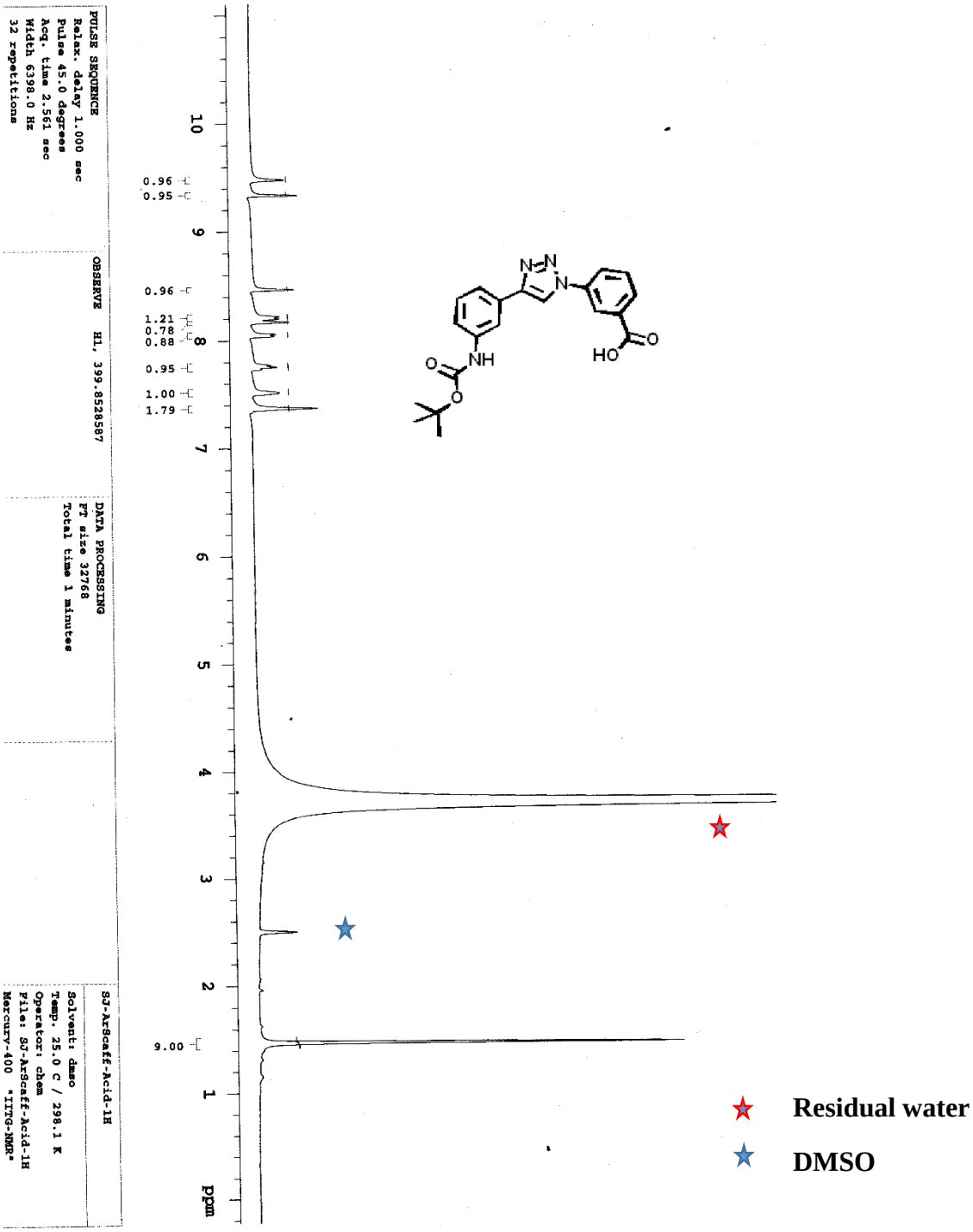


Figure S36. ^{1}H Spectra of synthesized compound **1.**

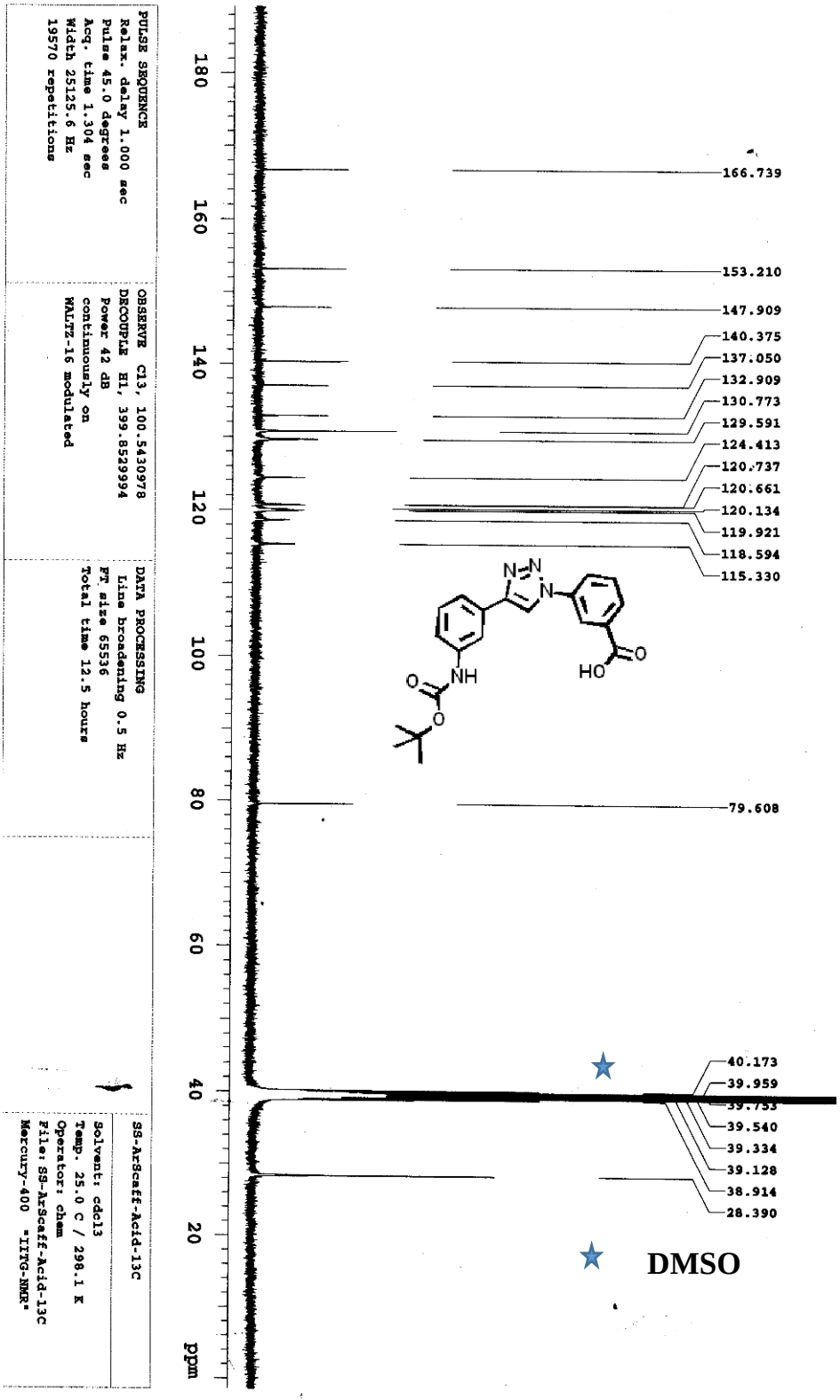


Figure S37. ^{13}C Spectra of synthesized compound **1.**

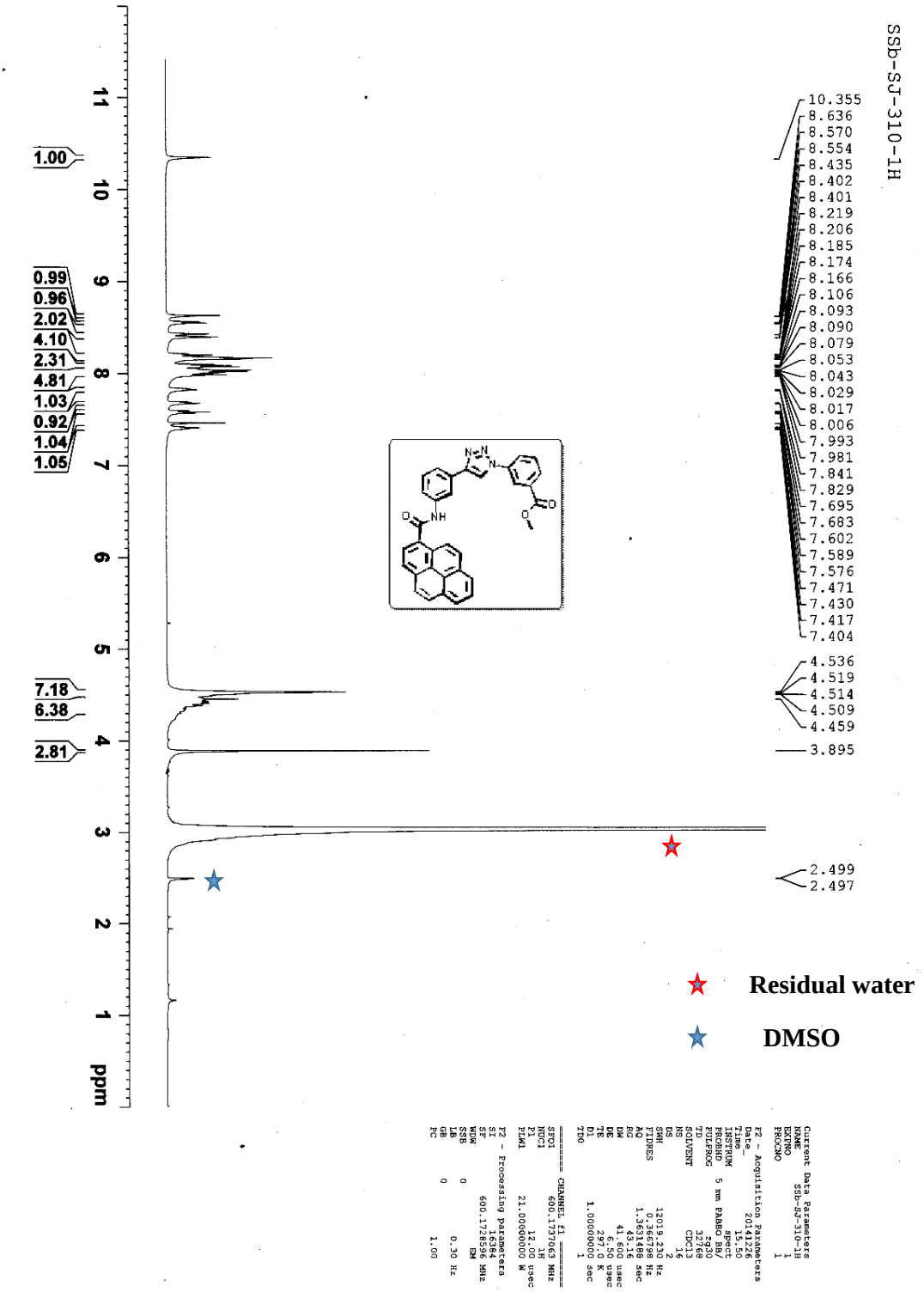


Figure S38. ^{1}H Spectra of synthesized compound **2.**

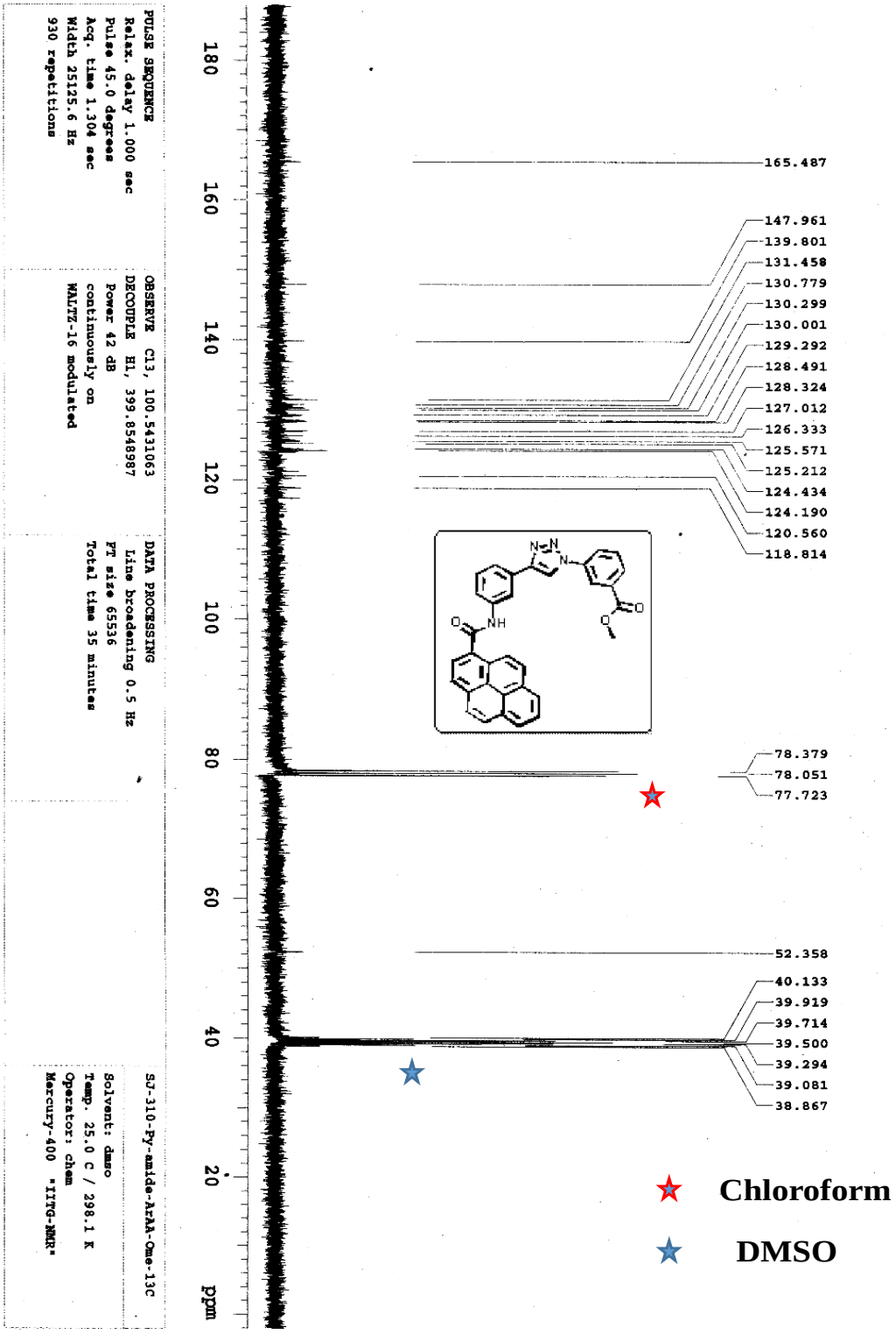


Figure S39. ^{13}C Spectra of synthesized compound **2.**

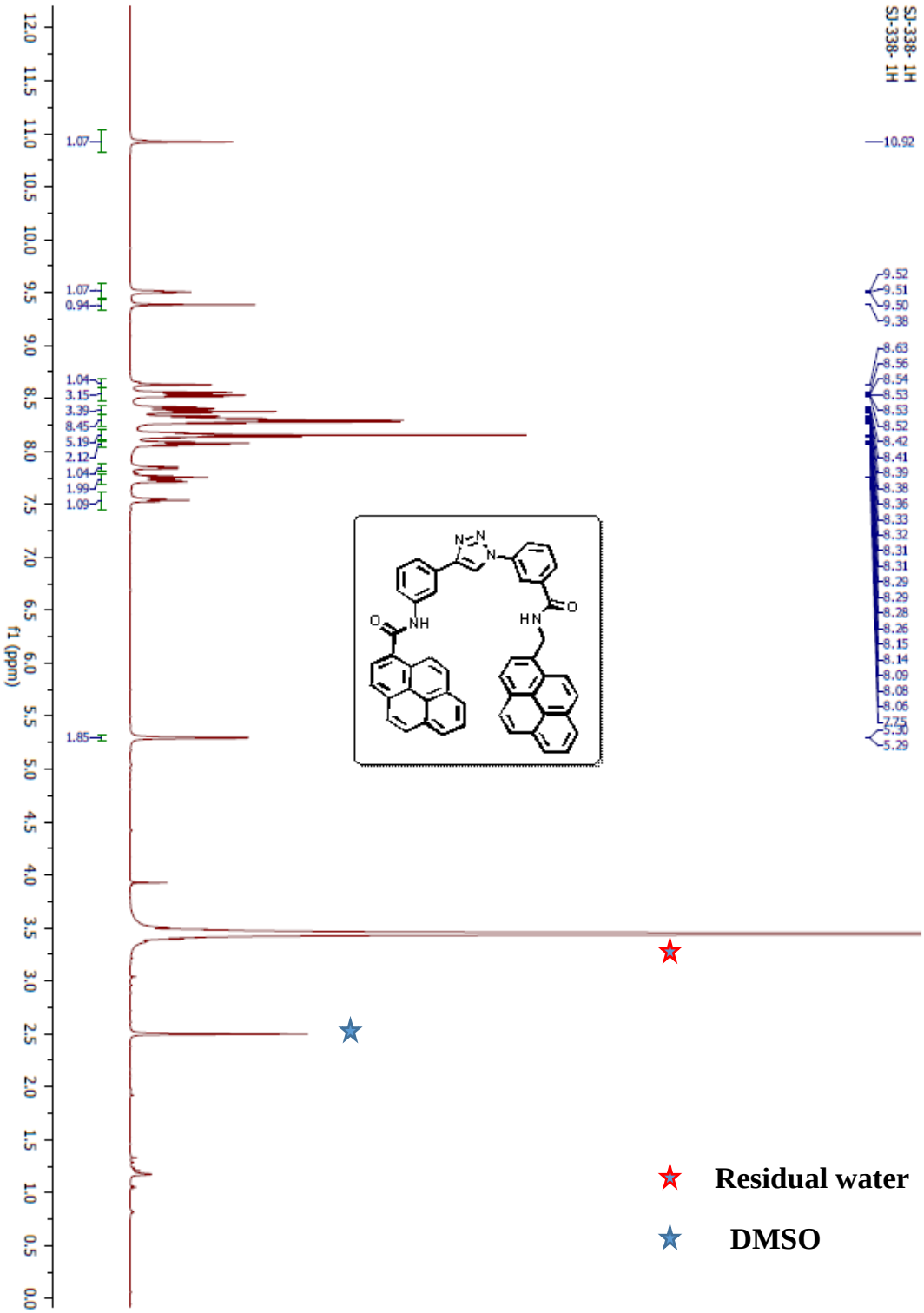


Figure S40. ^{1}H Spectra of synthesized compound **3.**

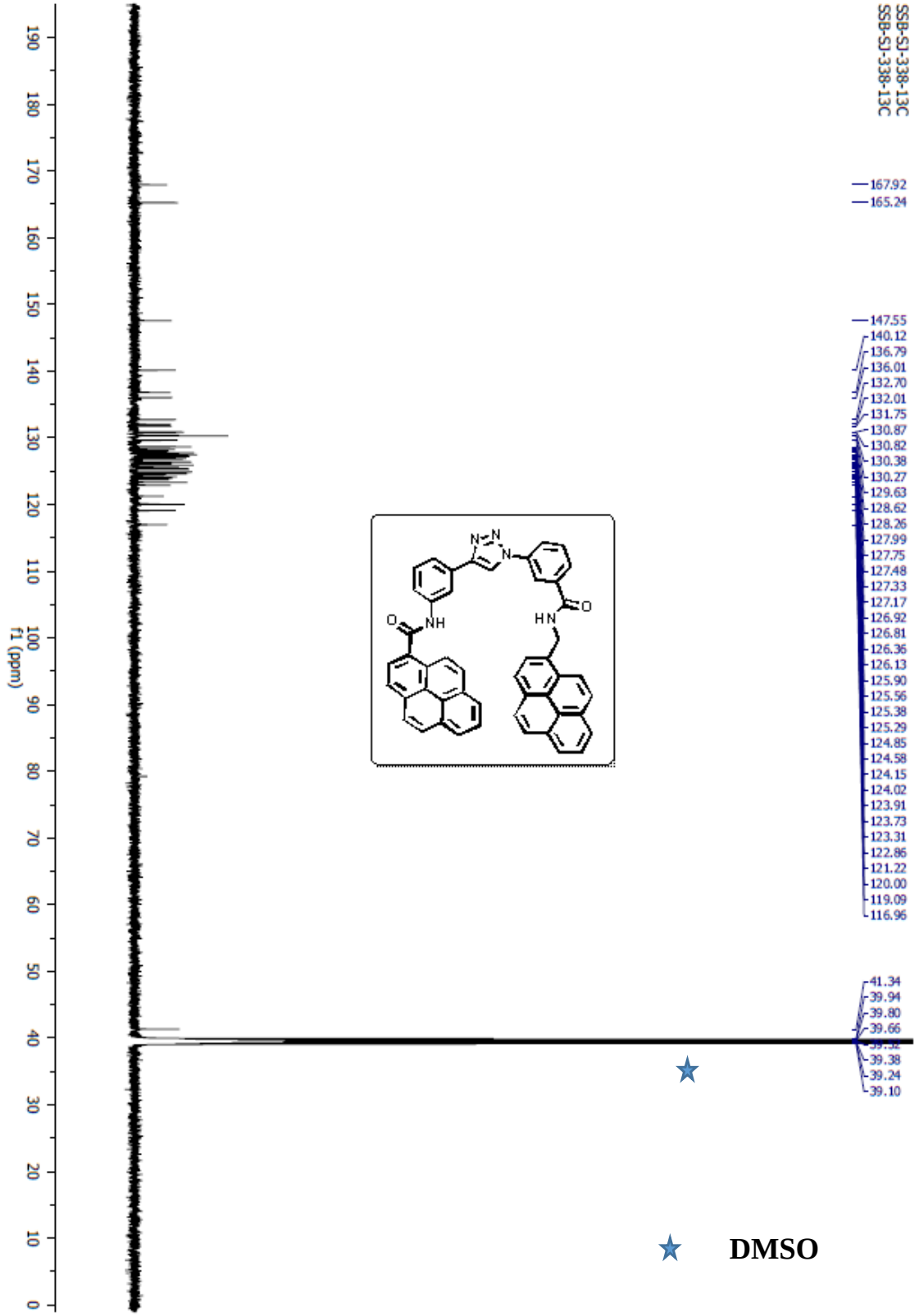


Figure S41. ^{13}C Spectra of synthesized compound **3.**

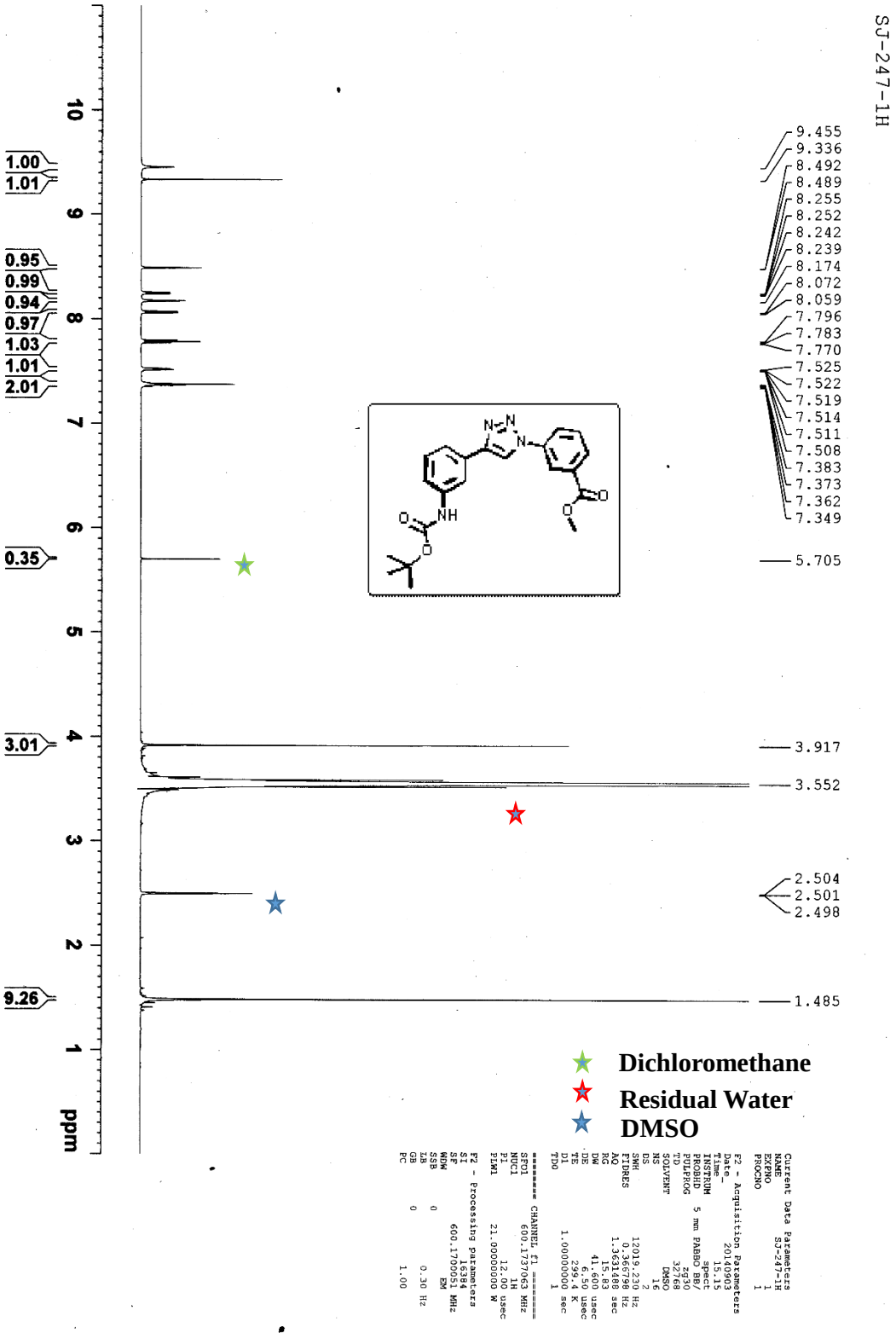


Figure S42. ^{1}H Spectra of synthesized compound **8.**

SSB-SJ-247-3-13C

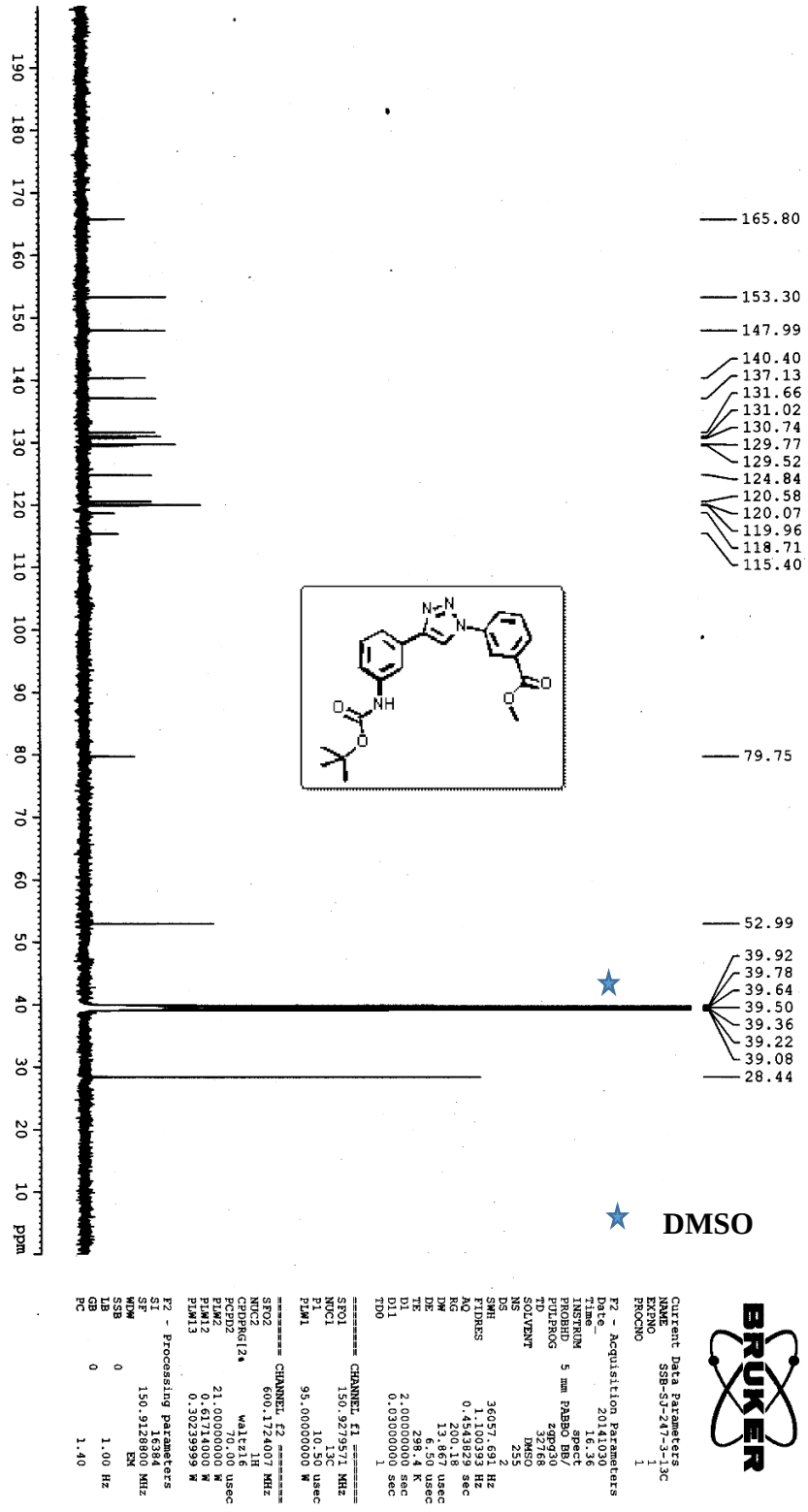


Figure S43. ^{13}C Spectra of synthesized compound **8.**