Electronic Supplementary Material (ESI) for New Journal of Chemistry.


# Supporting Information

## A new imidazole based phenanthridine probe for ratiometric fluorescent monitoring of methanol in biodiesel

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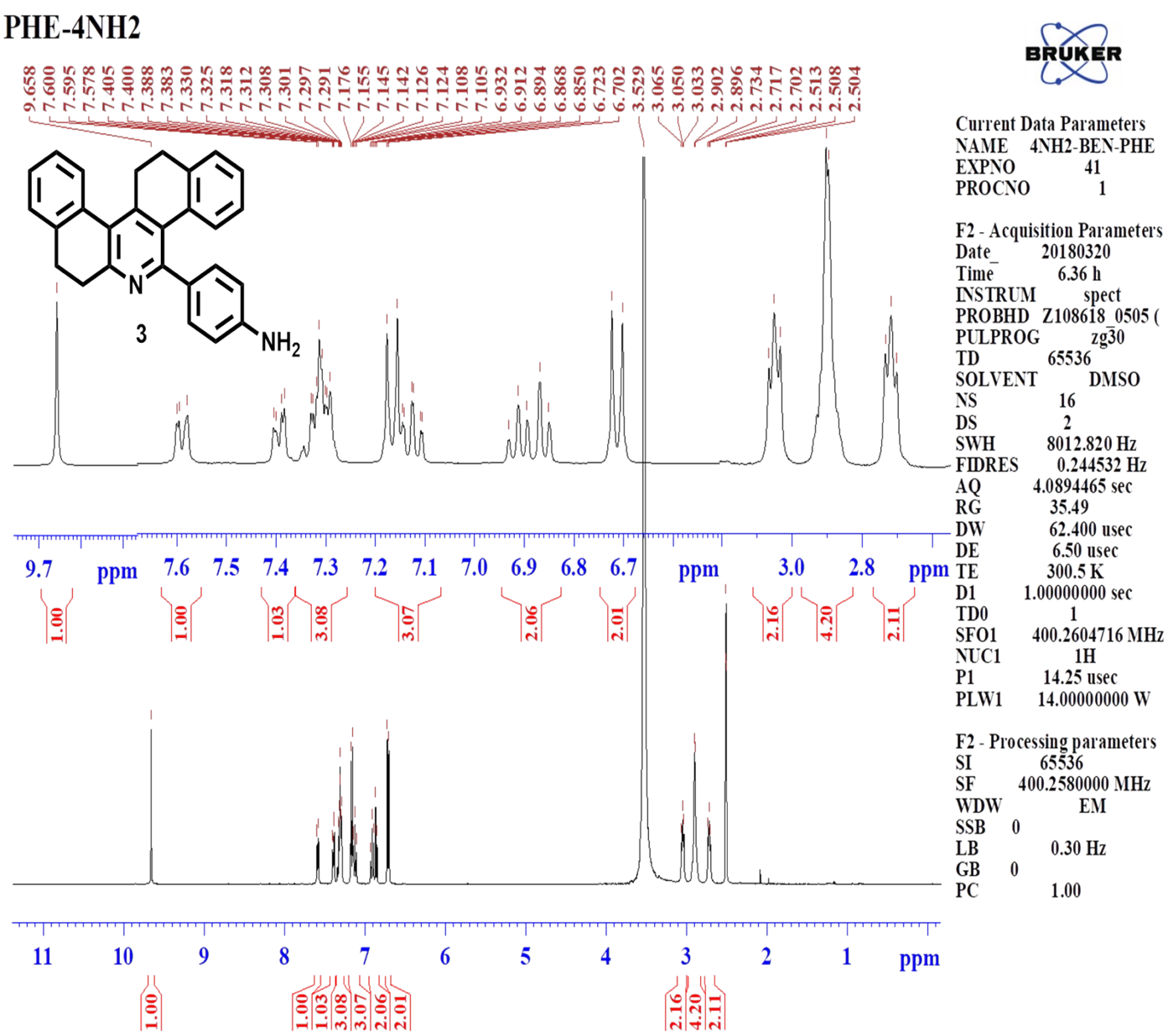



**Figure-S1.** $^{1}$H NMR (400 MHz, DMSO) spectra of compound **3**

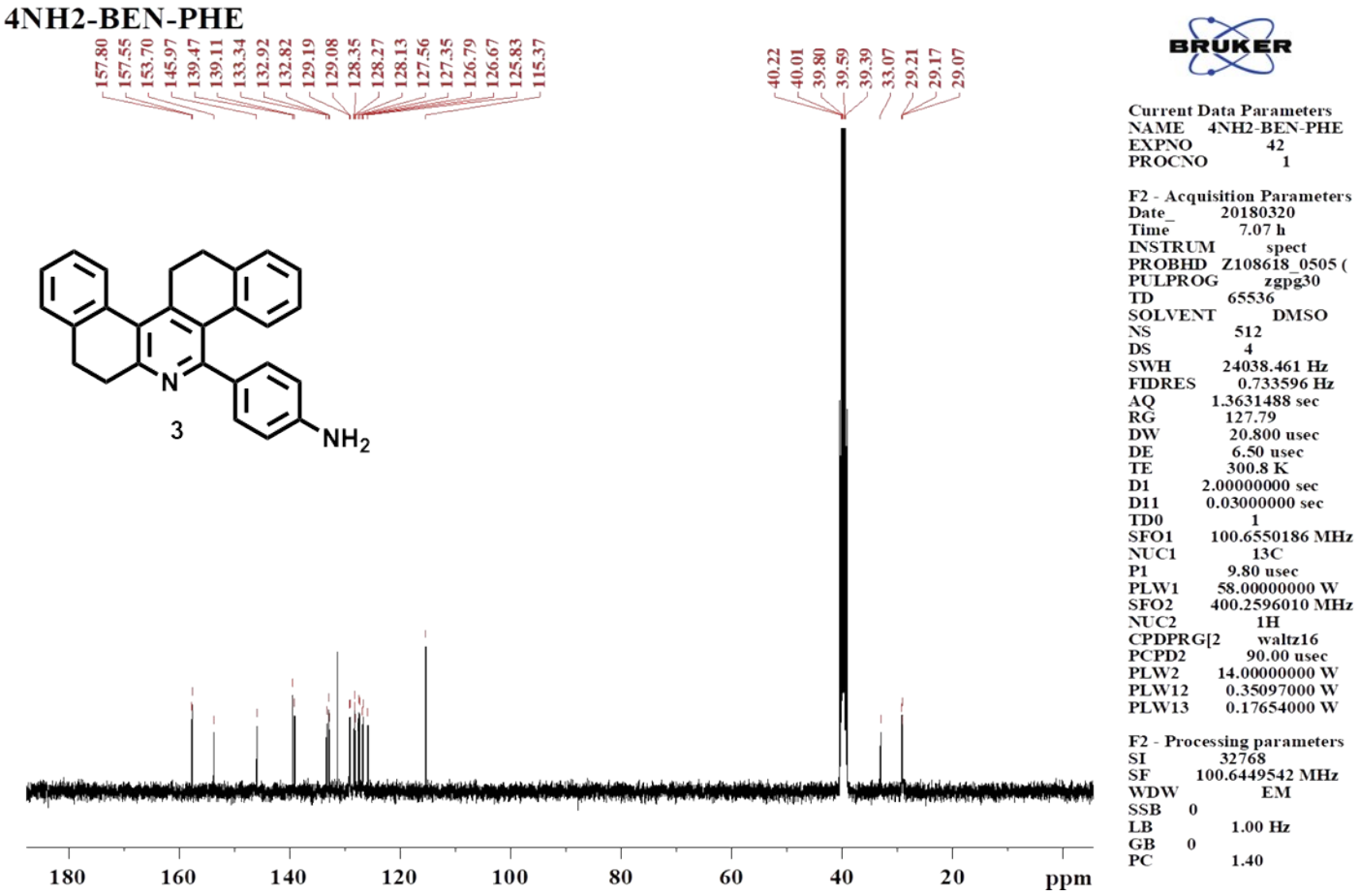



**Figure-S2.** $^{13}$C NMR (100 MHz, DMSO) spectra of compound **3**

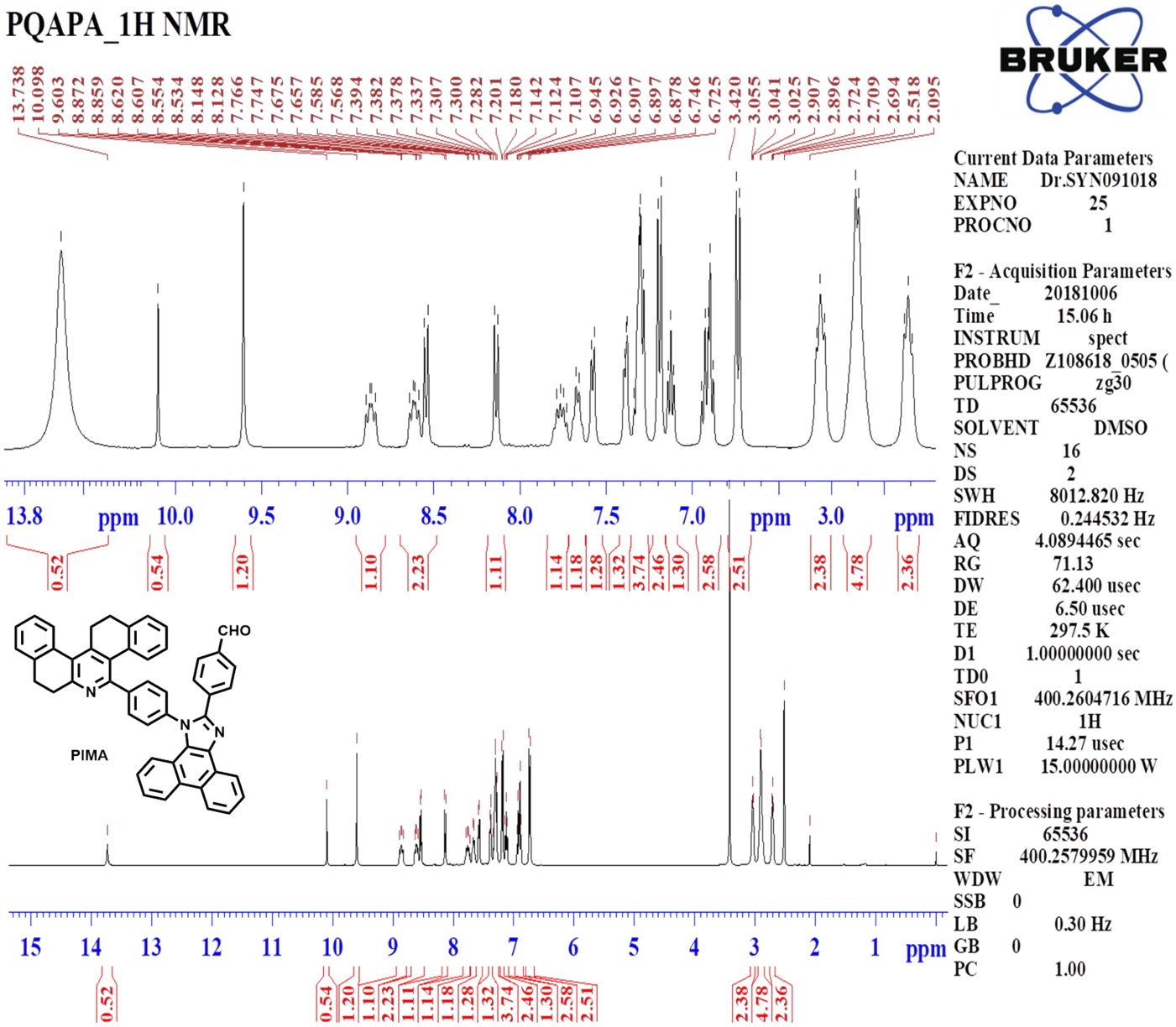



**Figure-S3.** $^{1}$H NMR (400 MHz, DMSO) spectra of compound **7**

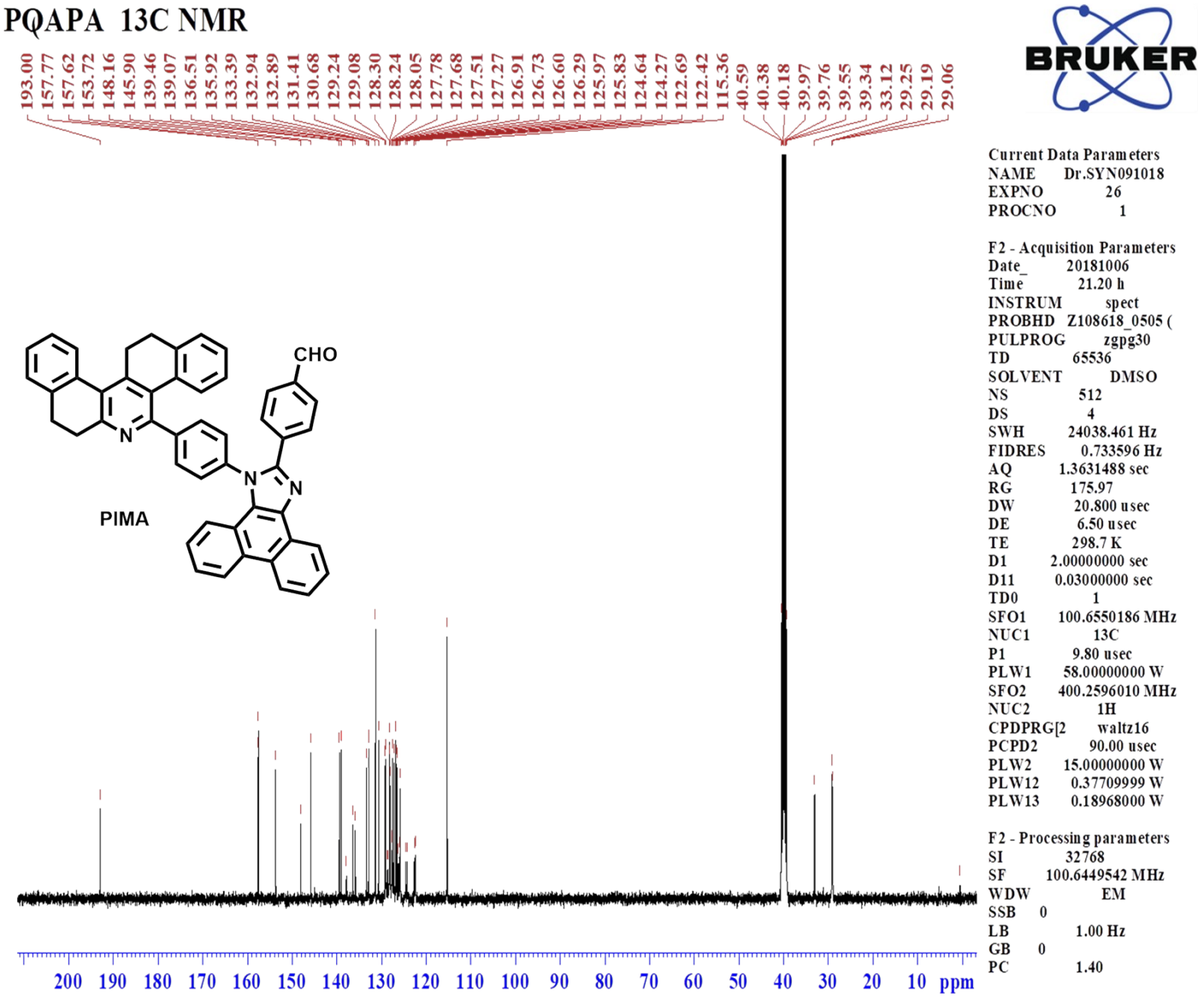



**Figure-S4.** $^{13}$C NMR (100 MHz, DMSO) spectra of compound **7**

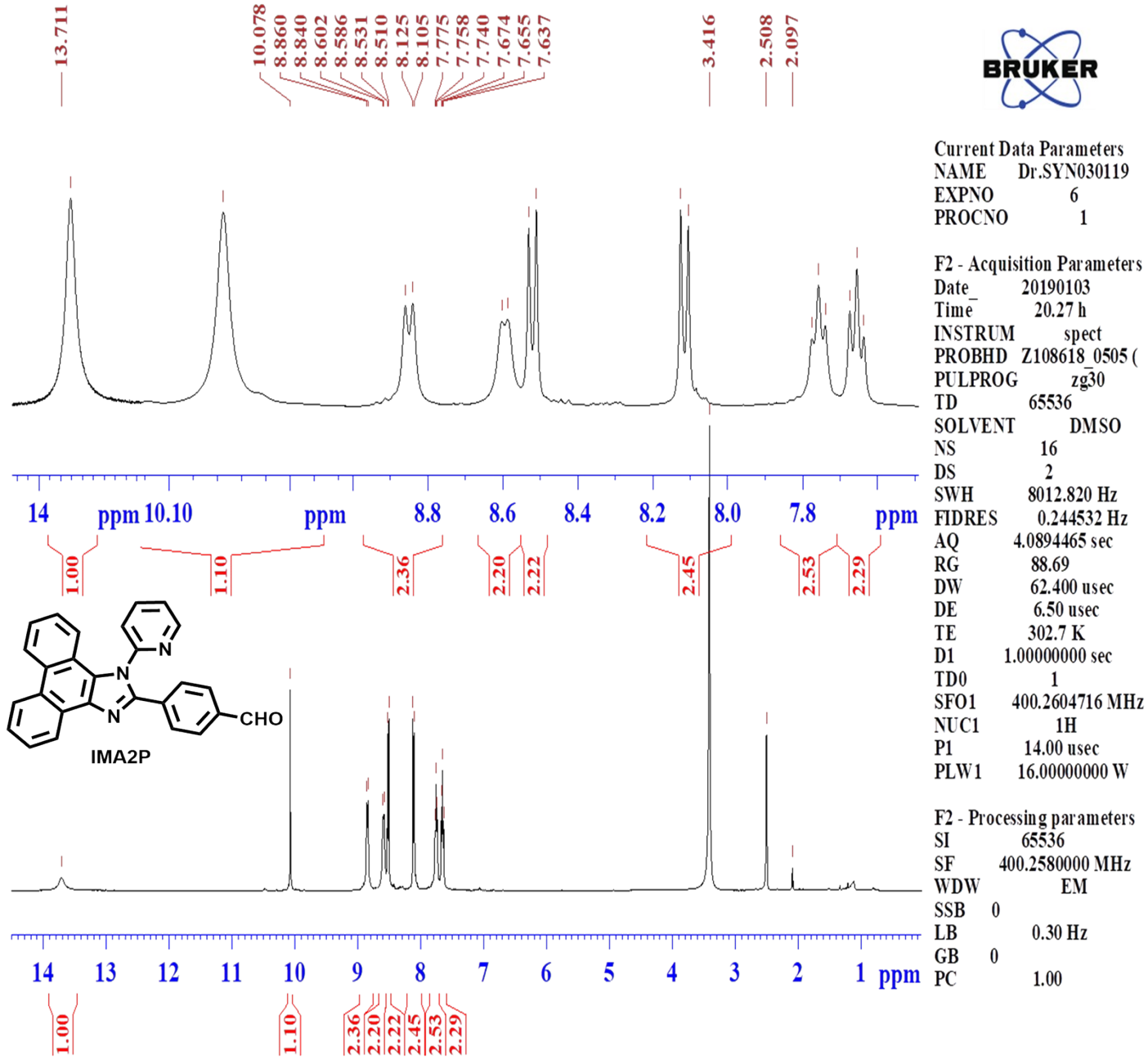



**Figure-S5.** [1]H NMR (400 MHz, DMSO) spectra of compound **9a**

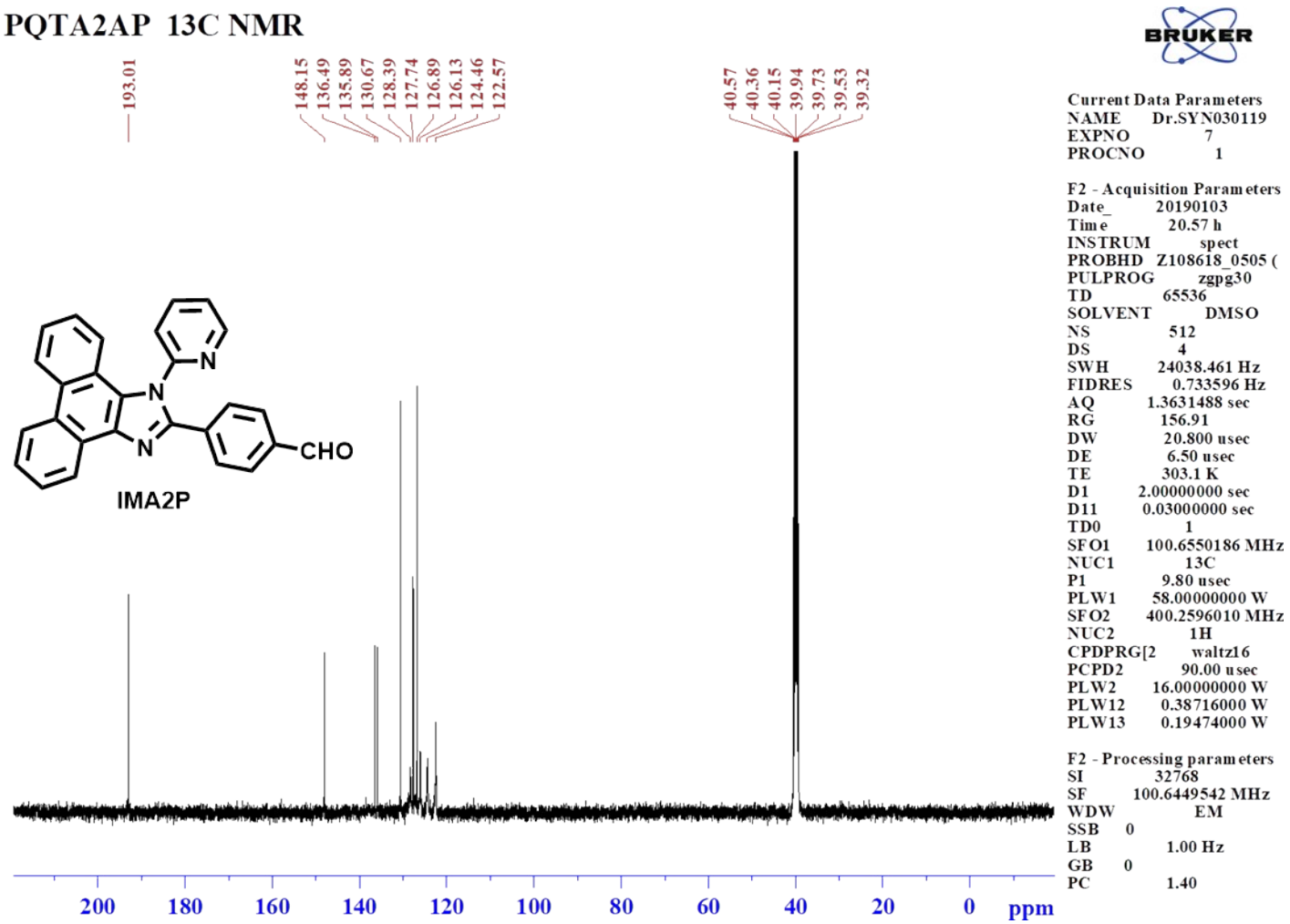



**Figure-S6.** $^{13}$C NMR (100 MHz, DMSO) spectra of compound **9a**

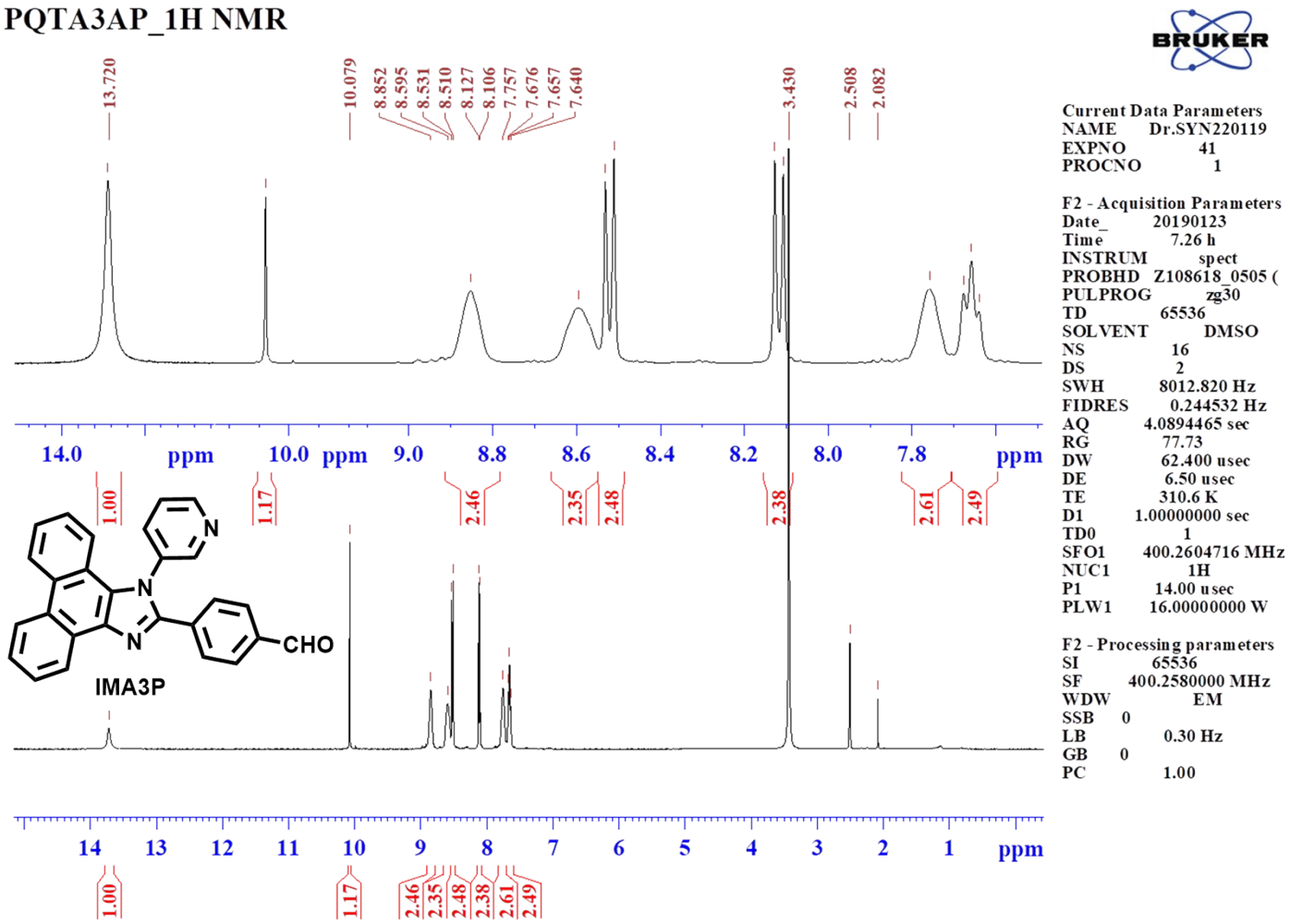



**Figure-S7.** $^{1}$H NMR (400 MHz, DMSO) spectra of compound **9b**

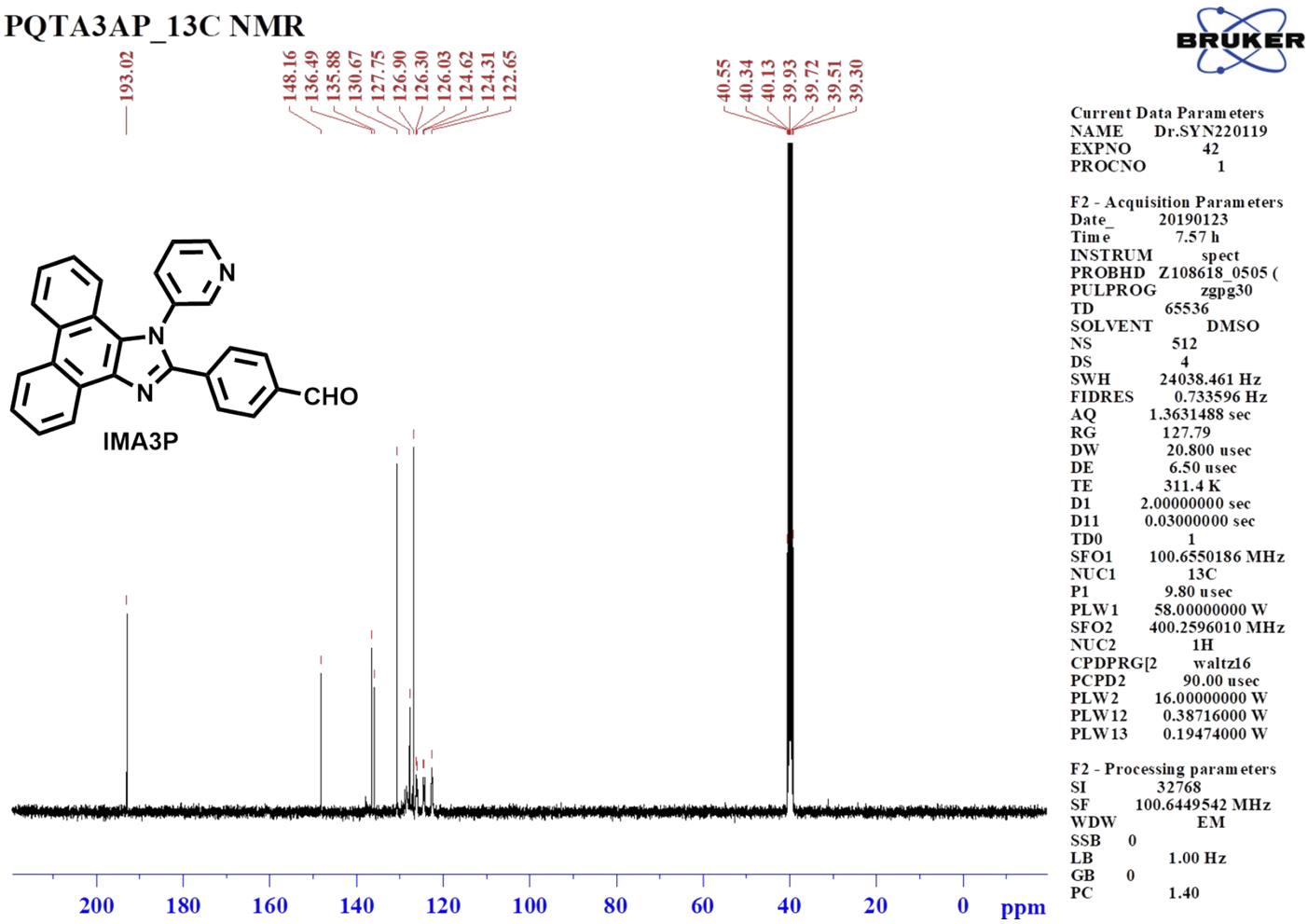



**Figure-S8.** $^{13}$C NMR (100 MHz, DMSO) spectra of compound **9b**

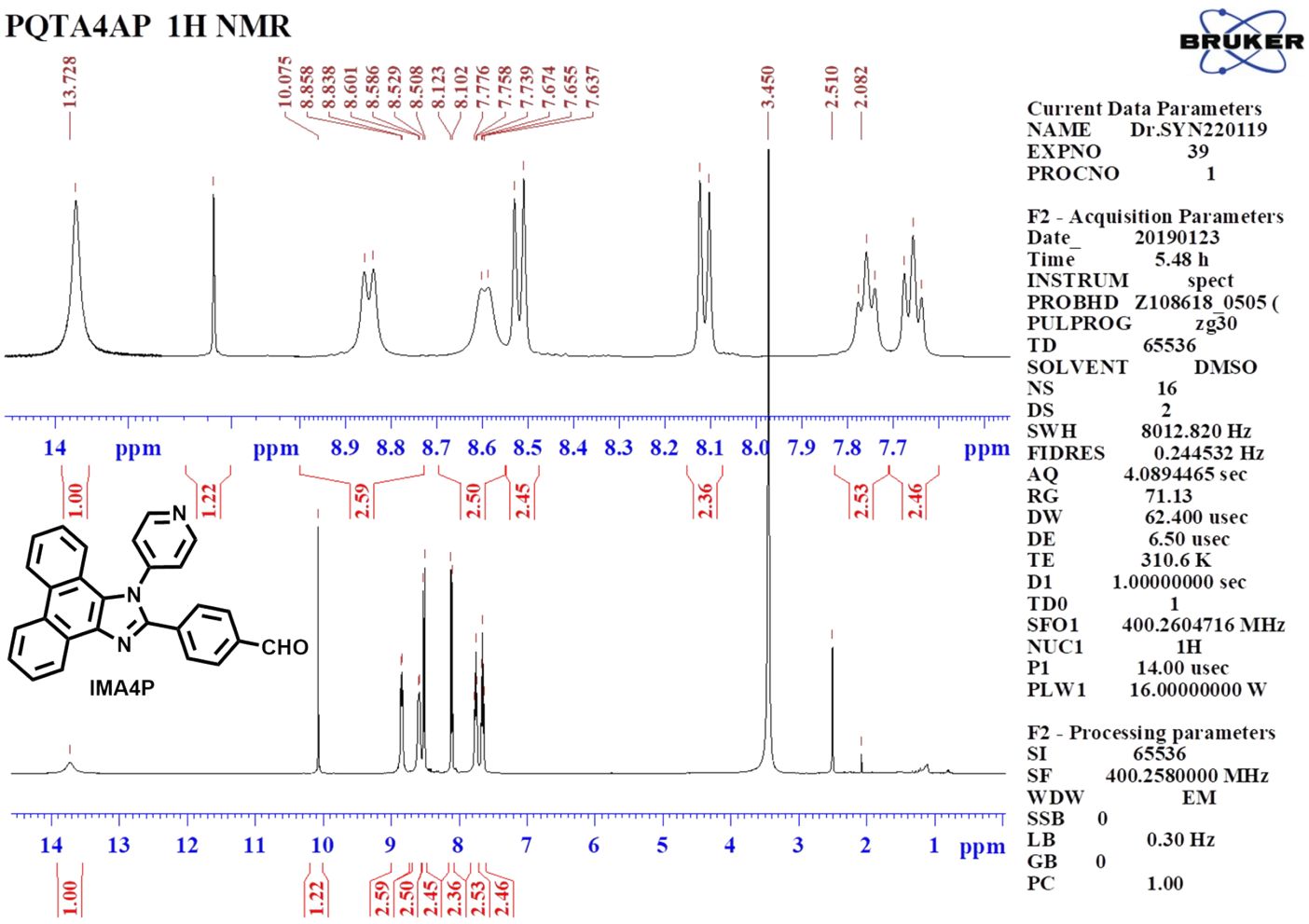



**Figure-S9.** $^{1}$H NMR (400 MHz, DMSO) spectra of compound **9c**

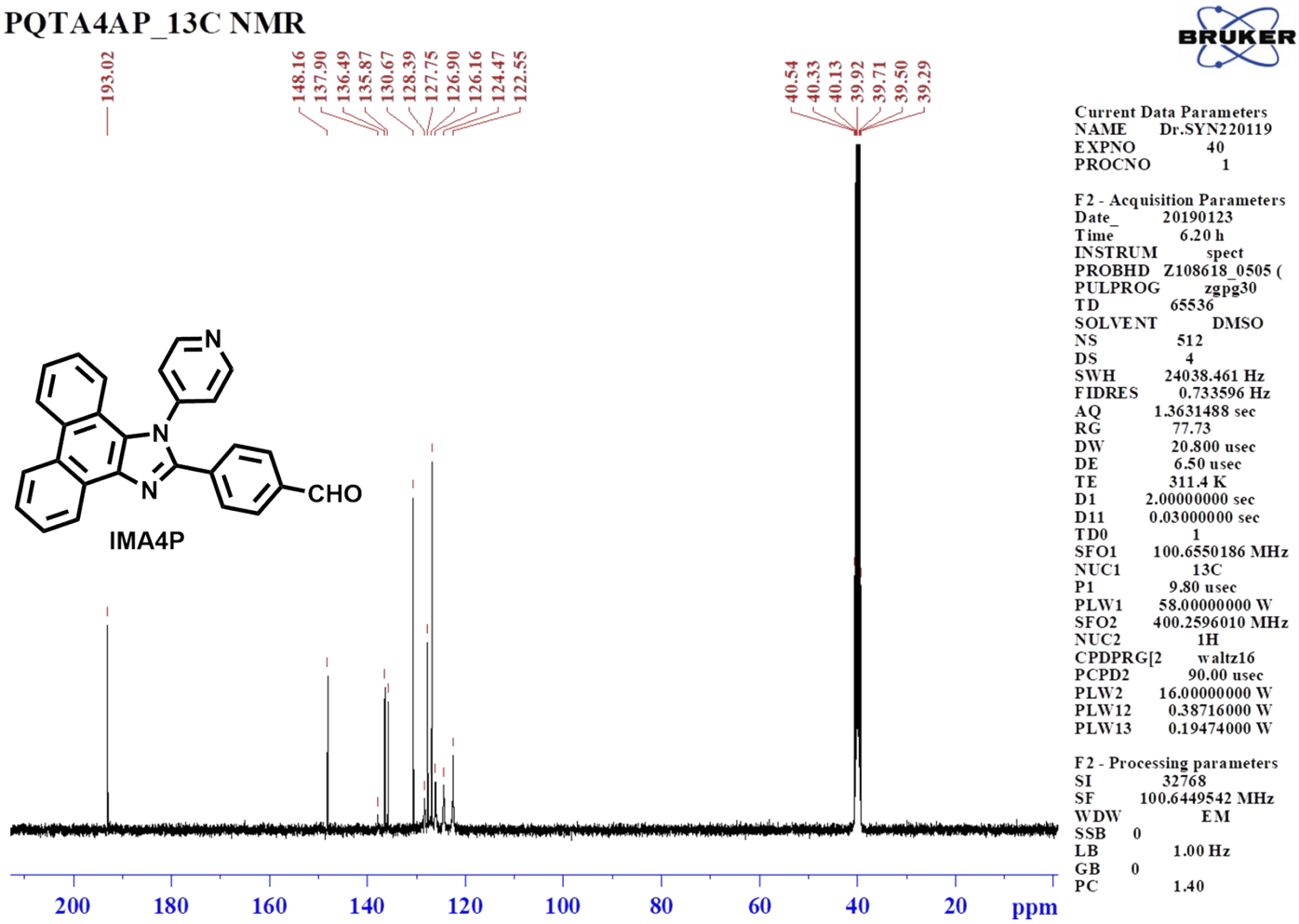



**Figure-S10.** $^{13}$C NMR (100 MHz, DMSO) spectra of compound **9c**

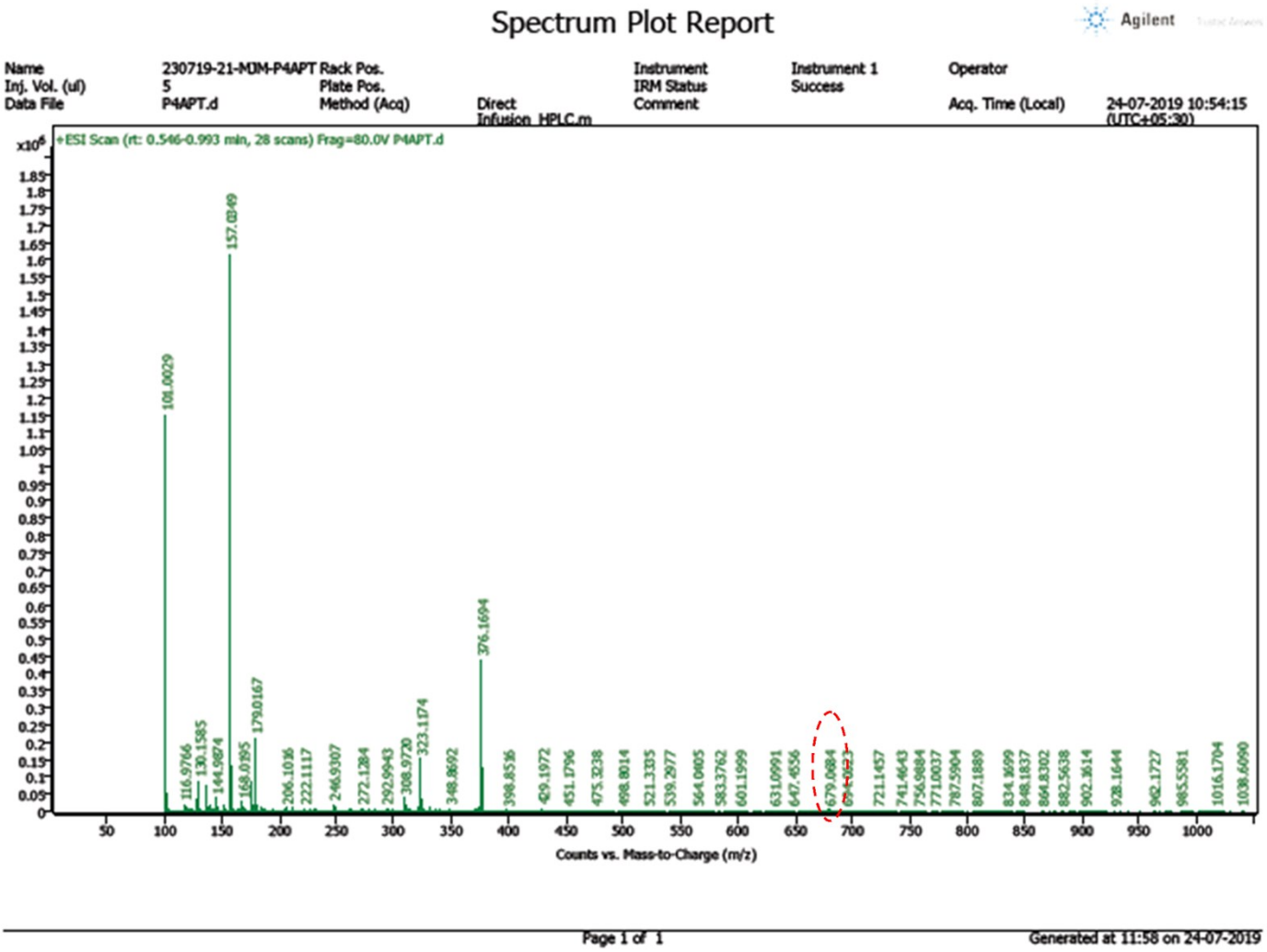



**Figure-S11.** ESI-MS spectra of compound of **7**

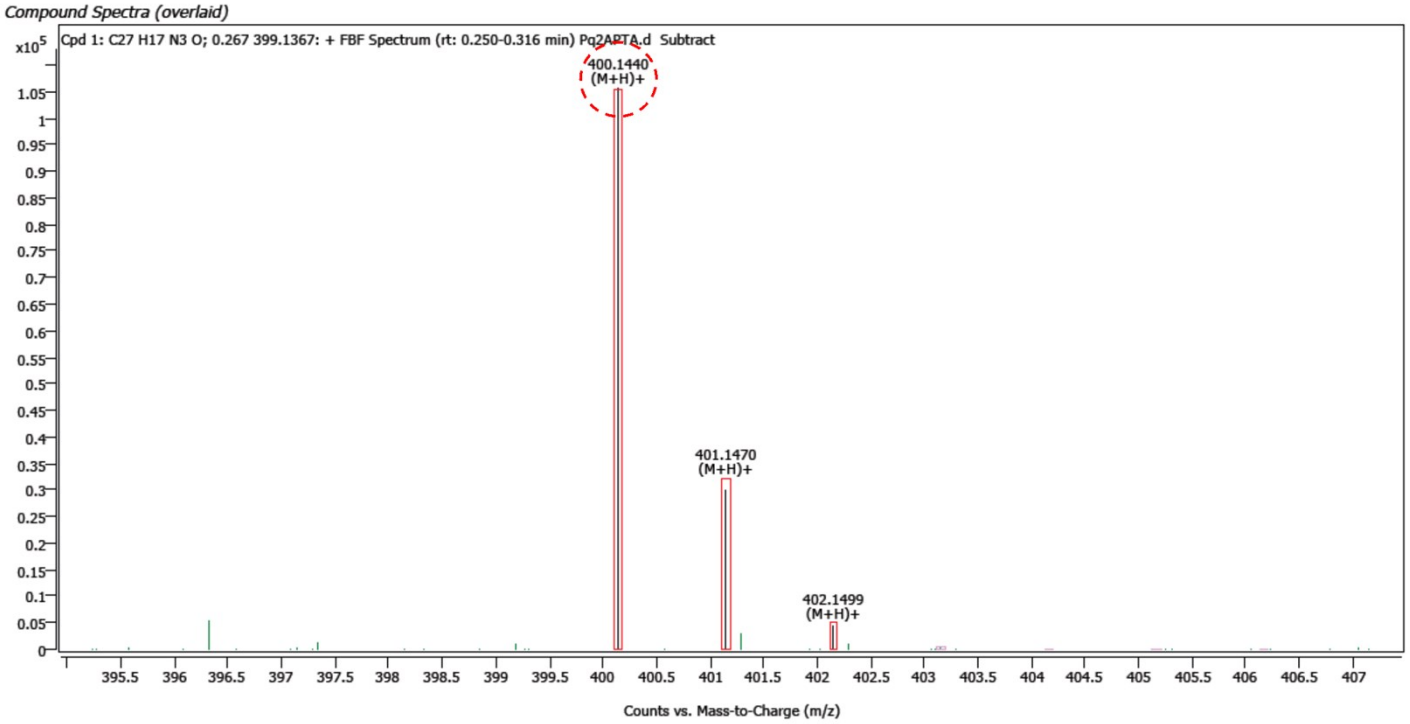
## ESI Mass Report

| | | | |
|---|---|---|---|
| **Name** | 230719-22-MJM-Pq2APTA | **Data File Path** | D:\MassHunter\Data\2019\JULY-2019\MJM\Pq2APTA.d |
| **Sample ID** | | **Acq. Time (Local)** | 24-07-2019 10:57:26 (UTC+05:30) |
| **Instrument** | Instrument 1 | **Method Path (Acq)** | D:\MassHunter\Methods\Direct Infusion_HPLC.m |
| **MS Type** | QTOF | **Version (Acq SW)** | 6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0) |
| **Inj. Vol. (ul)** | 5 | **IRM Status** | Success |
| **Position** | P2-E11 | **Method Path (DA)** | D:\MassHunter\Methods\10.0\IIT-Target Screening_1.m |
| **Plate Pos.** | | **Target Source Path** | |
| **Operator** | | **Result Summary** | 1 qualified (1 targets) |

## Compound Details

**Cpd. 1: C27 H17 N3 O**

*Compound Spectra (overlaid)*




*Compound ID Table*

| Cpd | Formula | Mass (Tgt) | Calc. Mass | Mass | Species | Diff(Tgt.ppm) | mDa |
|---|---|---|---|---|---|---|---|
| 1 | C27 H17 N3 O | 399.1372 | 399.1367 | 400.1440 | (M+H)+ | -1.28 | -0.51 |

**Figure-S12.** ESI-MS spectra of compound of **9a**

## ESI Mass Report

| | | | |
|---|---|---|---|
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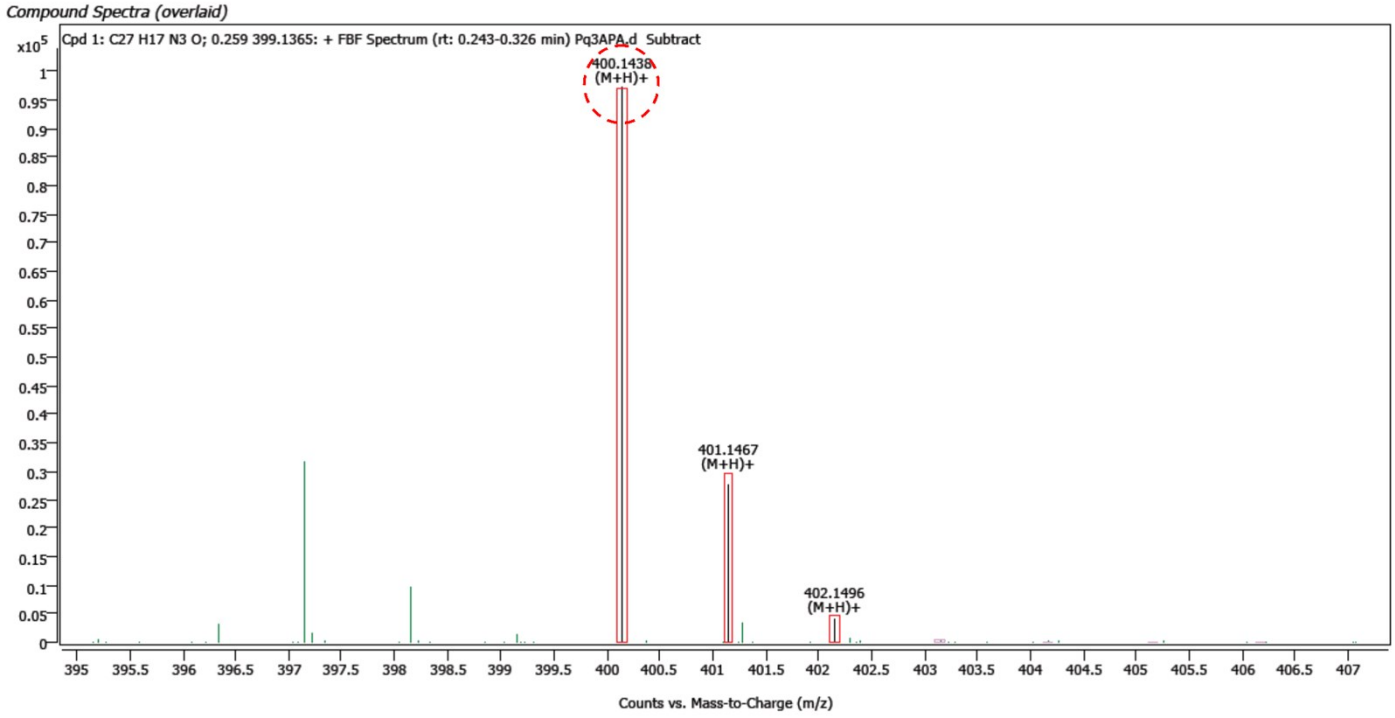
| **MS Type** | QTOF | **Version (Acq SW)** | 6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0) |
| **Inj. Vol. (ul)** | 5 | **IRM Status** | Success |
| **Position** | P2-F1 | **Method Path (DA)** | D:\MassHunter\Methods\10.0\IIT-Target Screening_1.m |
| **Plate Pos.** | | **Target Source Path** | |
| **Operator** | | **Result Summary** | 1 qualified (1 targets) |

### Compound Details

**Cpd. 1: C27 H17 N3 O**

*Compound Spectra (overlaid)*




*Compound ID Table*

| Cpd | Formula | Mass (Tgt) | Calc. Mass | Mass | Species | Diff(Tgt.ppm) | mDa |
|---|---|---|---|---|---|---|---|
| 1 | C27 H17 N3 O | 399.1372 | 399.1365 | 400.1438 | (M+H)+ | -1.71 | -0.68 |

**Figure-S13.** ESI-MS spectra of compound of **9b**

## ESI Mass Report

| | | | |
|---|---|---|---|
| **Name** | 230719-24-MJM-Pq4APTA | **Data File Path** | D:\MassHunter\Data\2019\JULY-2019\MJM\Pq4APTA.d |
| **Sample ID** | | **Acq. Time (Local)** | 24-07-2019 11:03:47 (UTC+05:30) |
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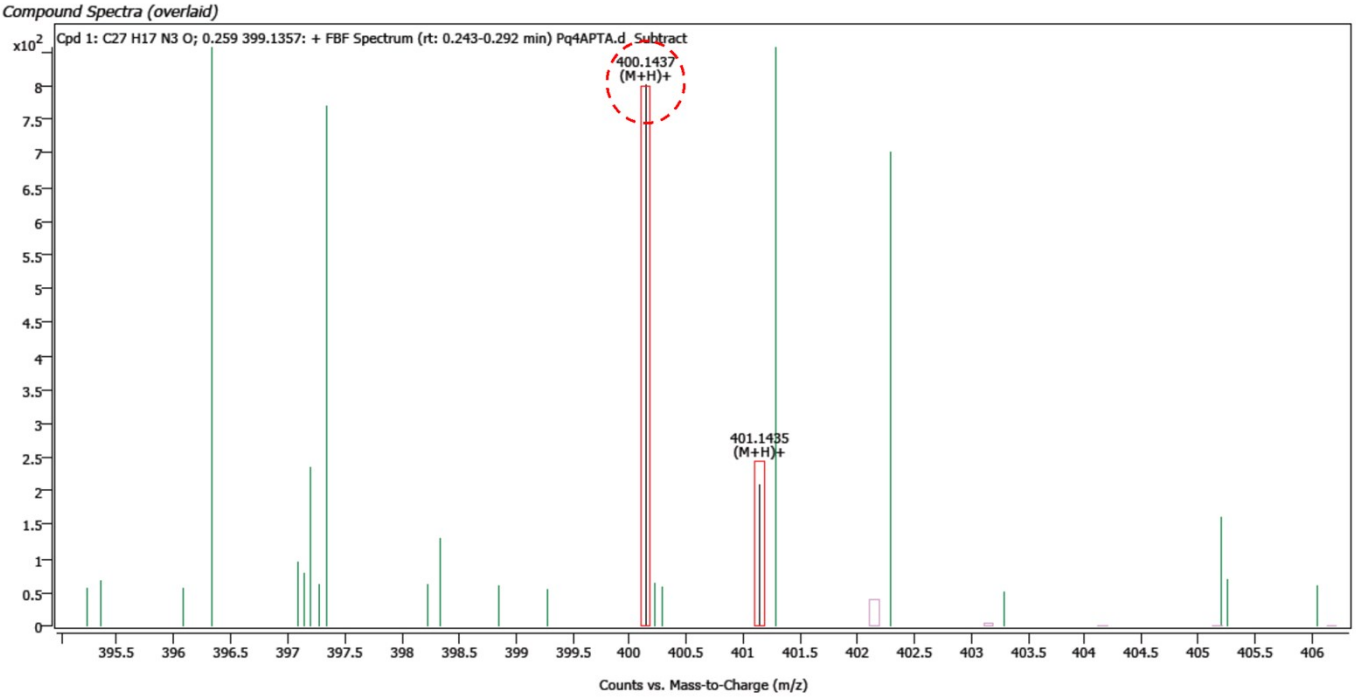
| **MS Type** | QTOF | **Version (Acq SW)** | 6200 series TOF/6500 series Q-TOF B.08.00 (B8058.0) |
| **Inj. Vol. (ul)** | 5 | **IRM Status** | Success |
| **Position** | P2-F2 | **Method Path (DA)** | D:\MassHunter\Methods\10.0\IIT-Target Screening_1.m |
| **Plate Pos.** | | **Target Source Path** | |
| **Operator** | | **Result Summary** | 1 qualified (1 targets) |

### Compound Details

**Cpd. 1: C27 H17 N3 O**

*Compound Spectra (overlaid)*




*Compound ID Table*

| Cpd | Formula | Mass (Tgt) | Calc. Mass | Mass | Species | Diff(Tgt.ppm) | mDa |
|---|---|---|---|---|---|---|---|
| 1 | C27 H17 N3 O | 399.1372 | 399.1357 | 400.1437 | (M+H)+ | -3.63 | -1.45 |

**Figure-S14.** ESI-MS spectra of compound of **9c**

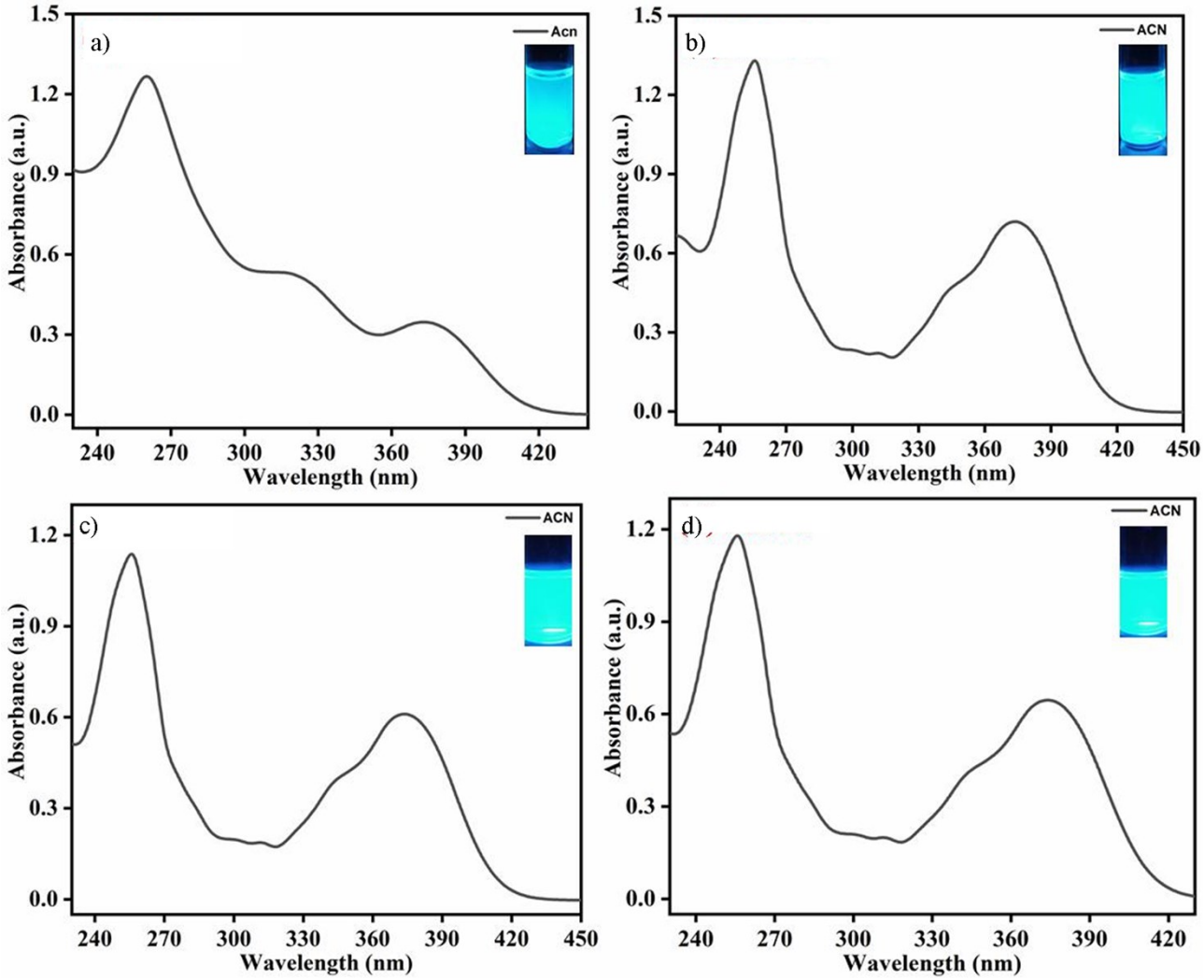
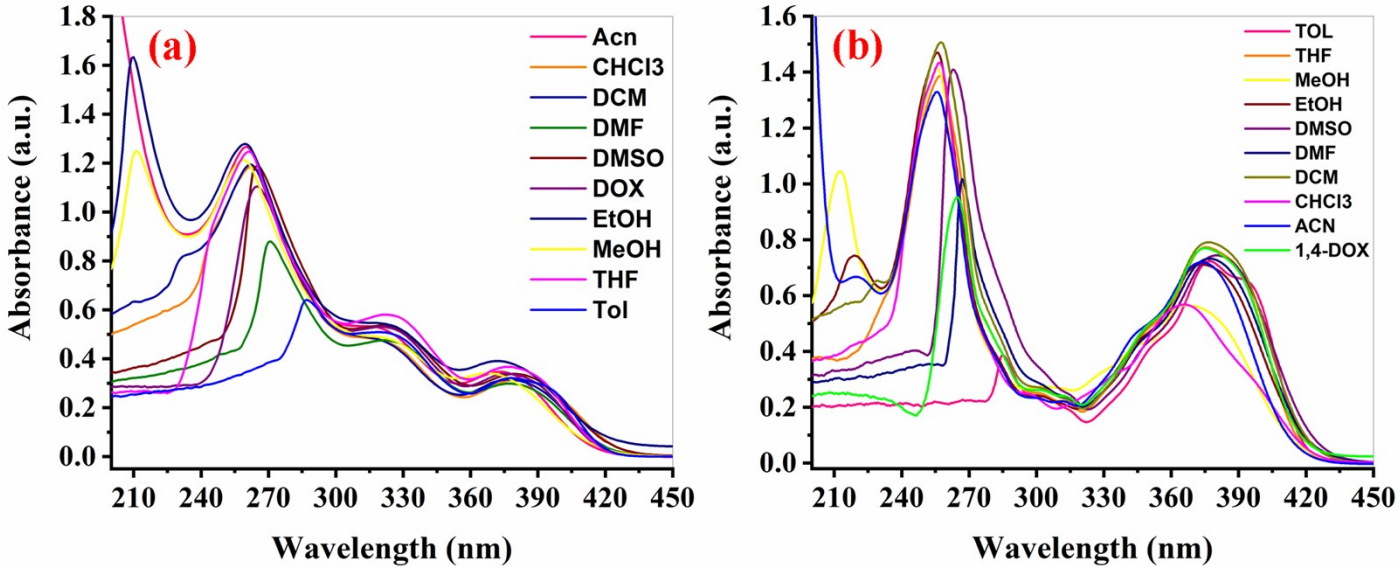



**Figure-S15.** UV spectra of compound of **7** (a), **9a** (b), **9b** (c), and **9c** (d) ($2x10^{-5}$) in Acetonitrile**.** Inset: compound of probs viewed under UV irradiation.



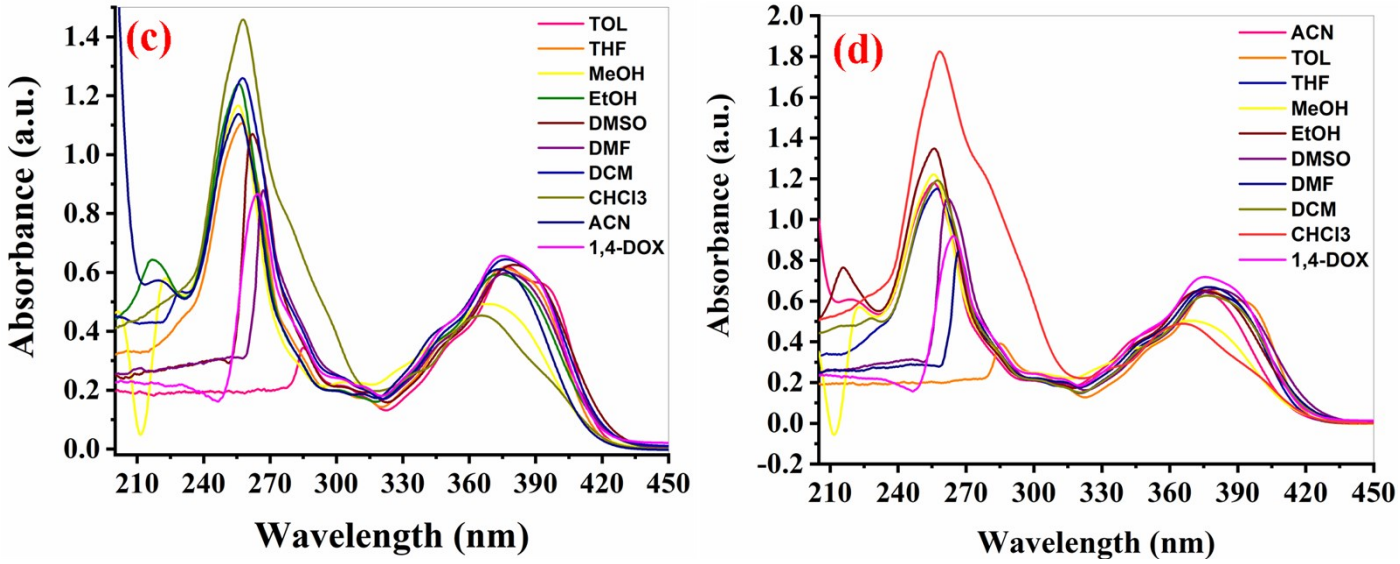



**Figure-S16** Absorbance spectra of compound **7** (a), **9a** (b), **9b** (c), and **9c** (d) ( $2x10^{-5}$) measured in different solvents

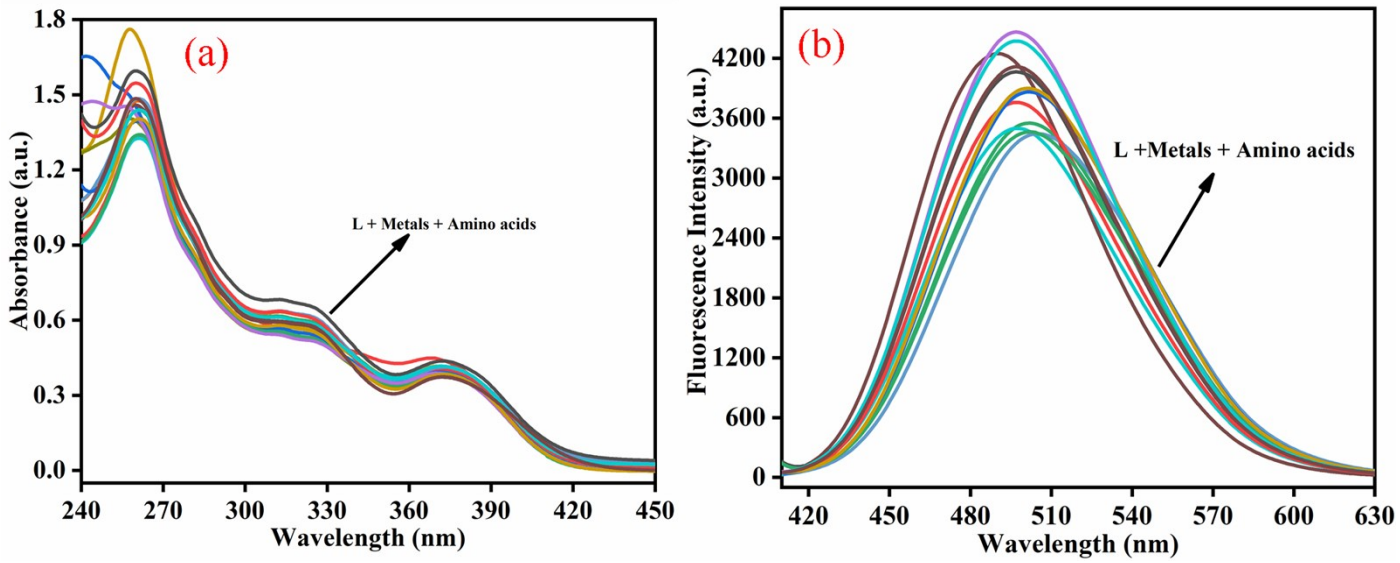



**Figure-S17.** Absorption spectra (a) and emission spectra (b) of compound **7** (**$2x10^{-5}$**) in the presence of various metal ions and amino acids ( $2x10^{-5}$).Similar to (**9a** , **9b**, and **9c)** following compounds

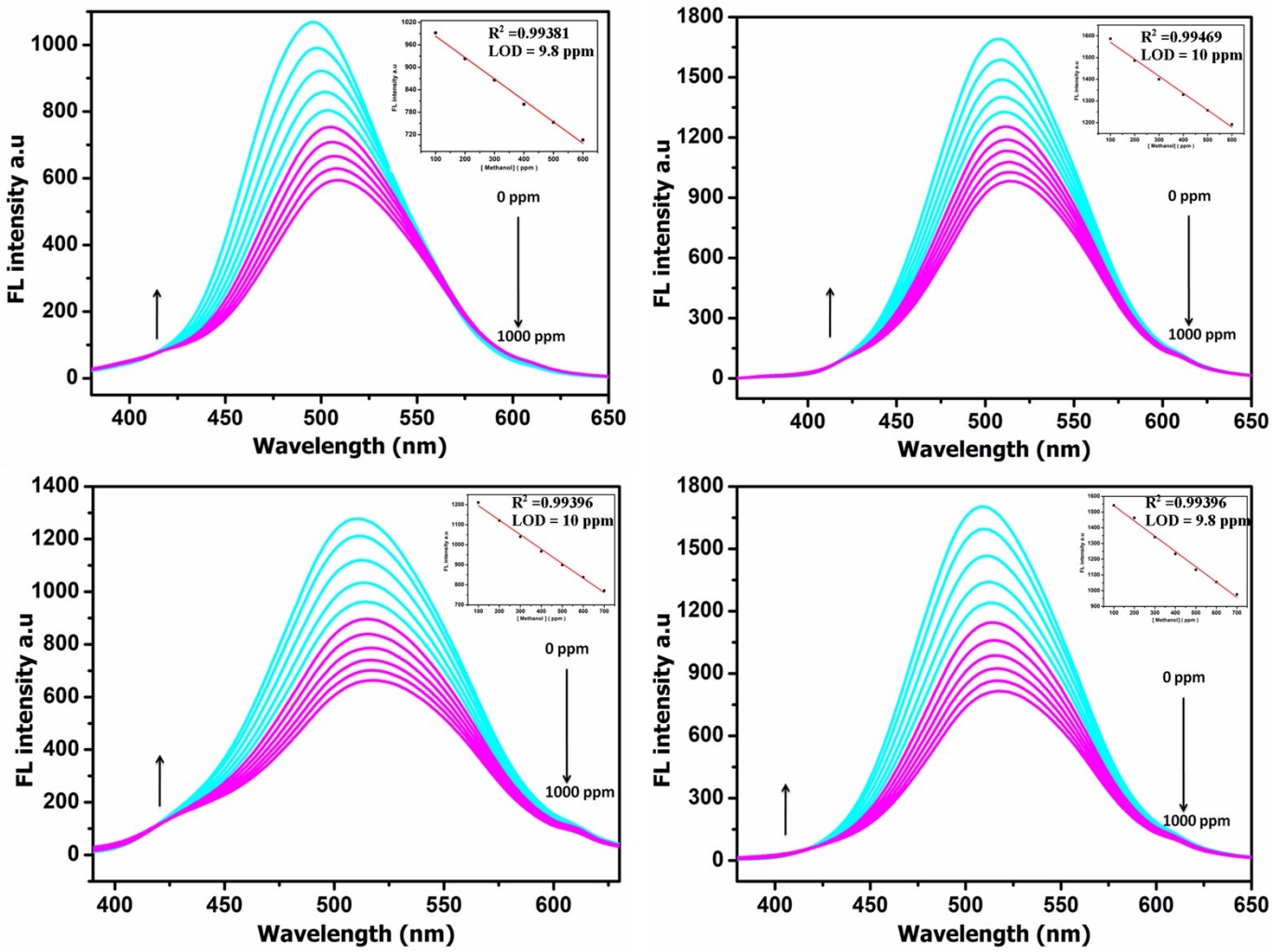
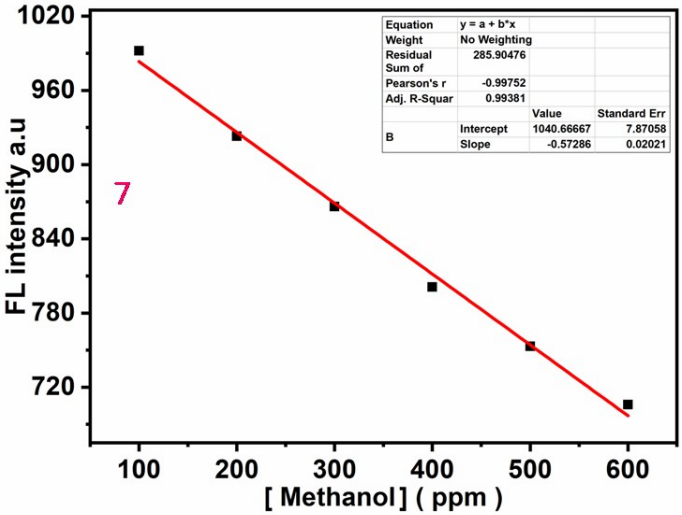



**Figure-S18.** Emission spectra of compound **7, 9a** , **9b**, and **9c** (**2x10**$^{-5}$) in the presence of methanol ( 0 to 1000ppm). Inset: linear relation between ligand (2x10$^{-5}$) and methanol concentration (0 to 1000ppm)



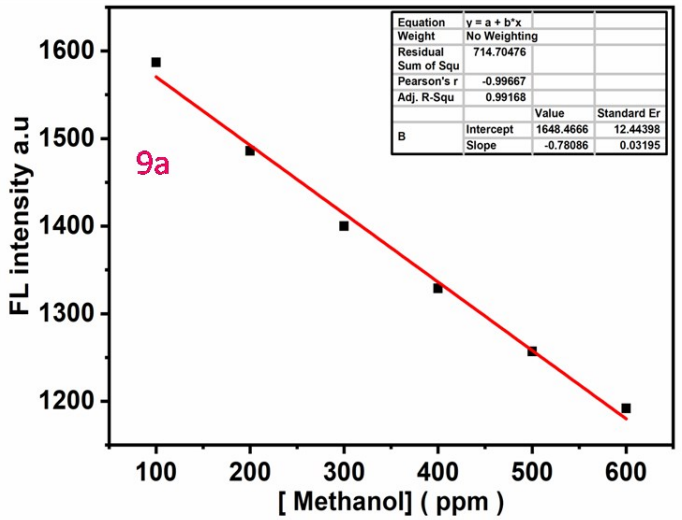

$$LOD = 3\sigma/K$$

$\sigma = 1.87$

$K = 0.5720 \times 10^{-6}$

$LOD = 3 \times 1.87 / 0.5720 \times 10^{-6}$

$LOD = 9.8$ ppm




$$LOD = 3\sigma/K$$

$\sigma = 2.70$

$K = 0.78086 \times 10^{-6}$

$LOD = 3 \times 2.70 / 0.78086 \times 10^{-6}$

$LOD = 10$ ppm

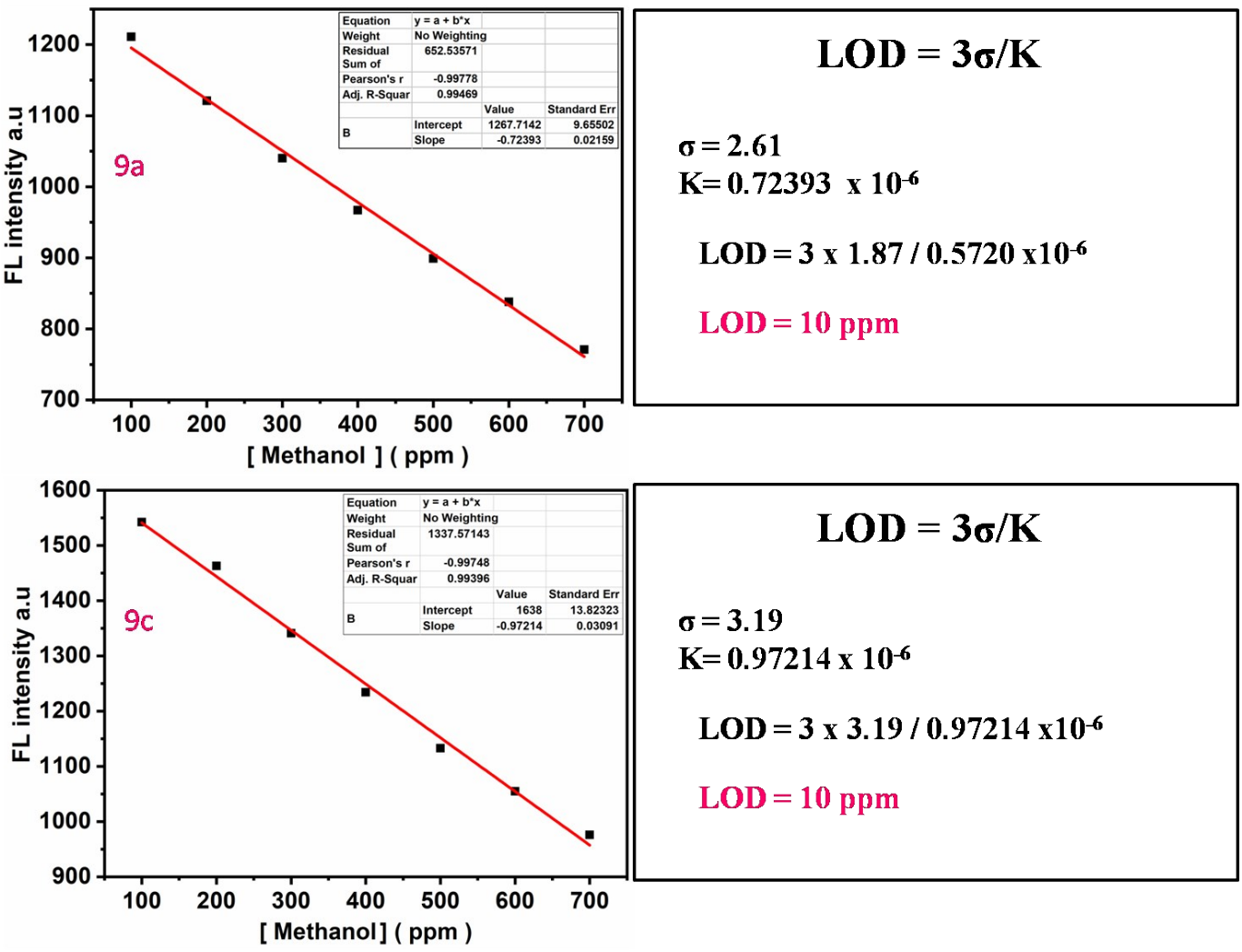



**Figure-S19** Plot of fluorescence intensity compounds of 7, 9a, 9b, 9c (at 438 nm) and the concentration of MeOH and the calculation of LOD

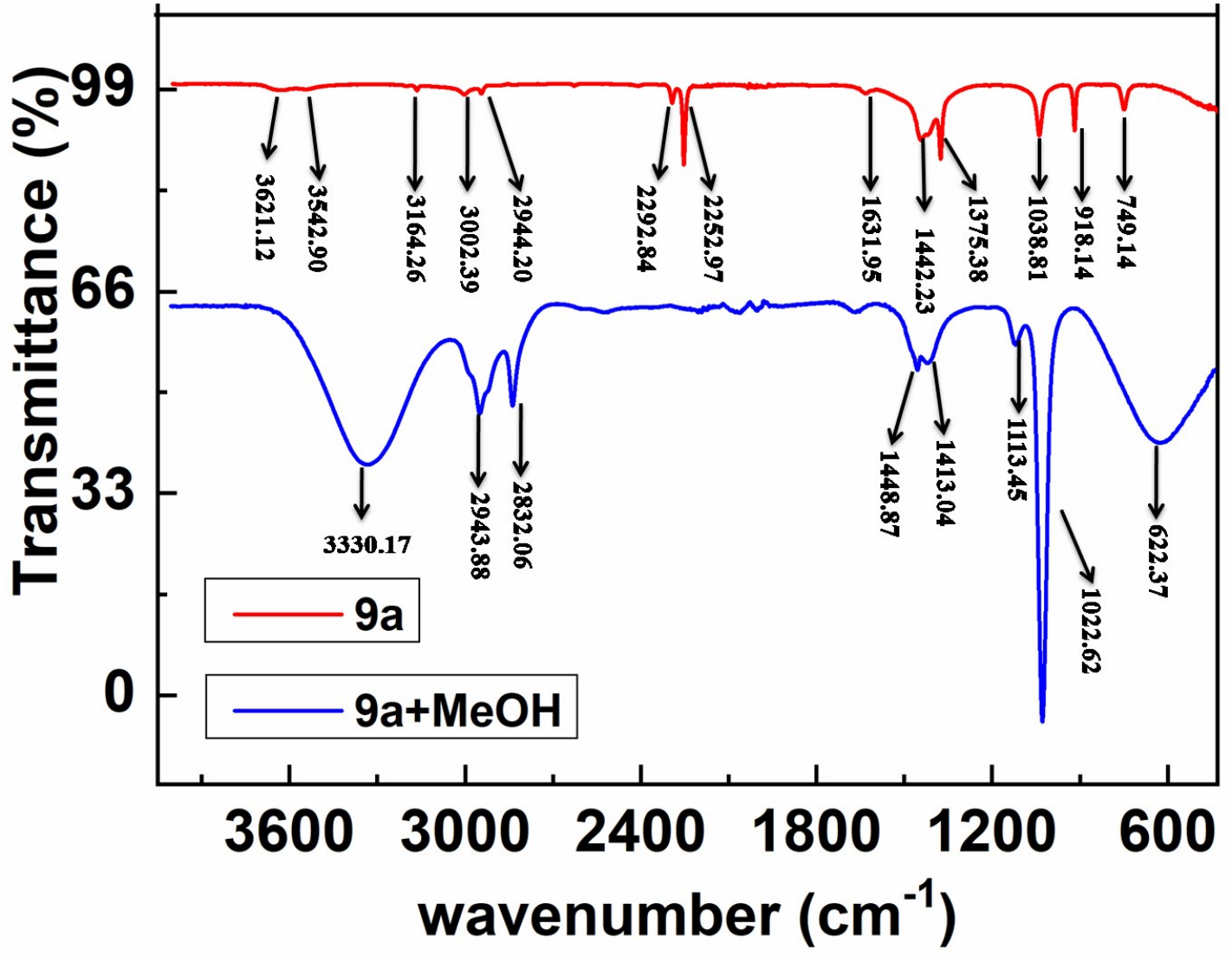



**Figure-S20** FTIR spectra of probe **9a** and **9a+MeOH**

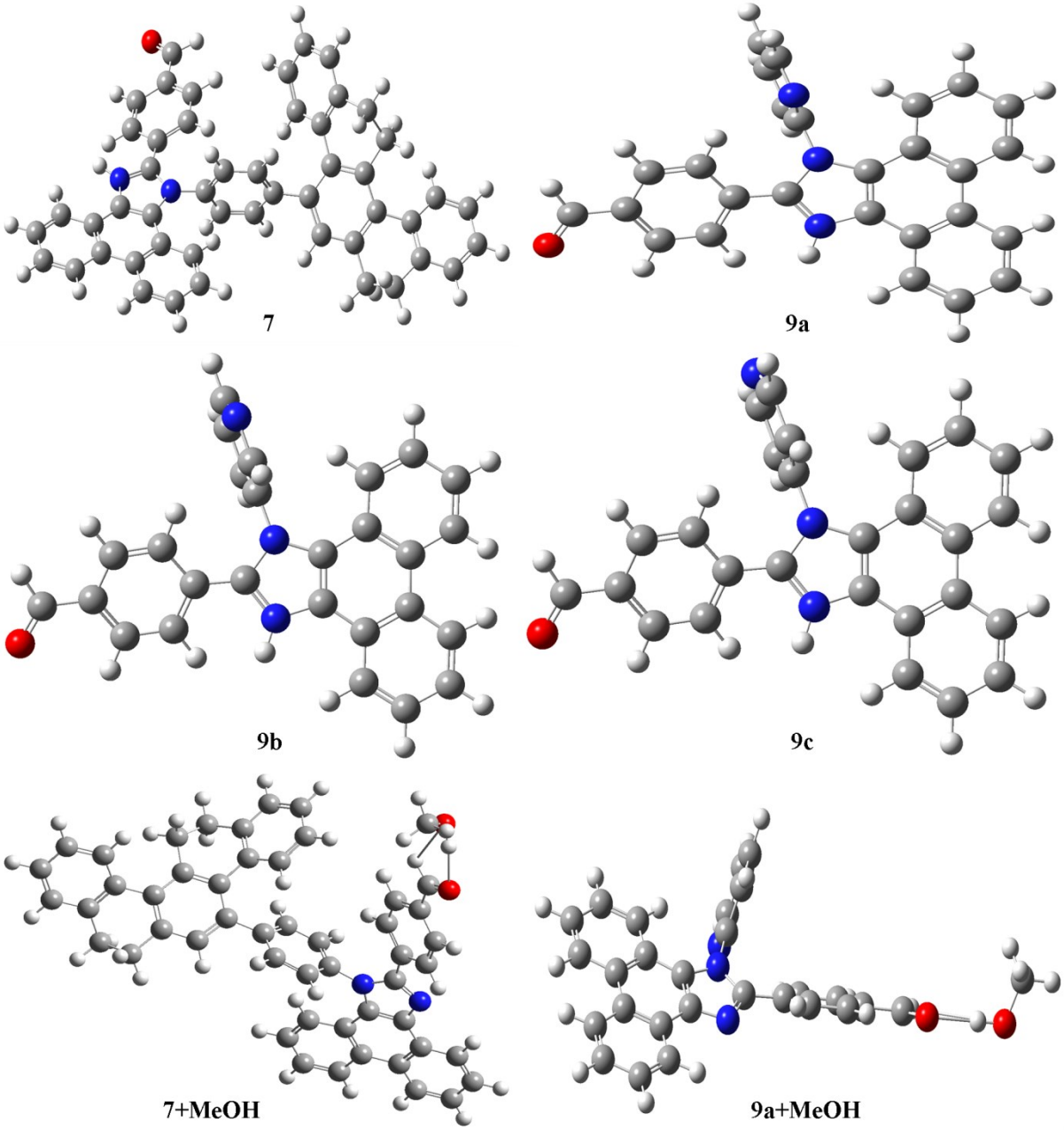
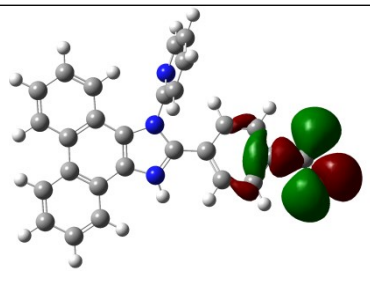
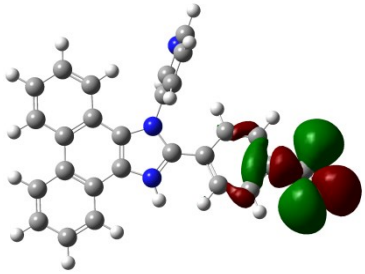
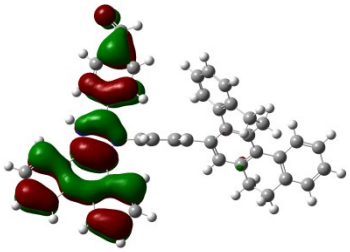
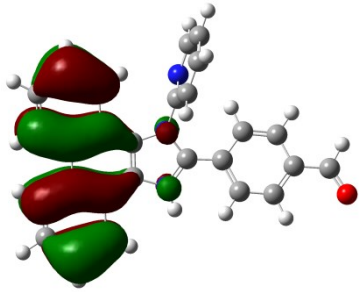
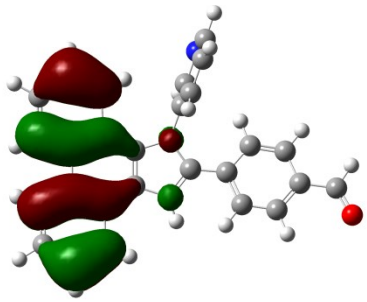
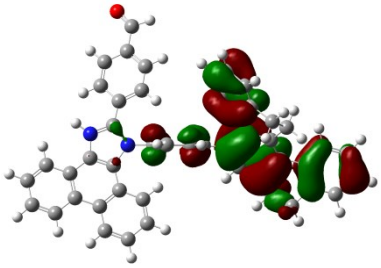
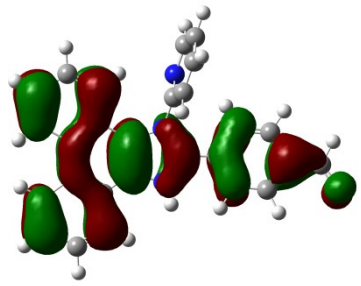
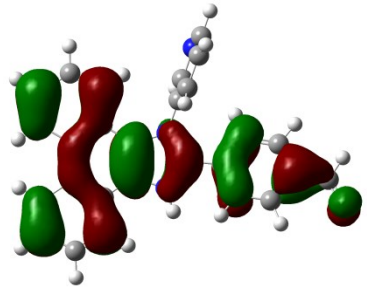
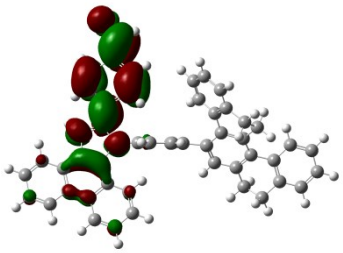
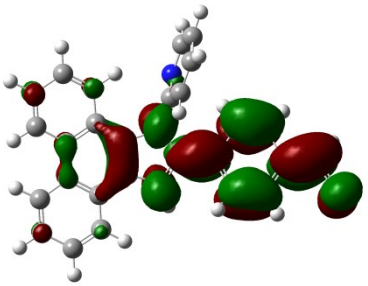
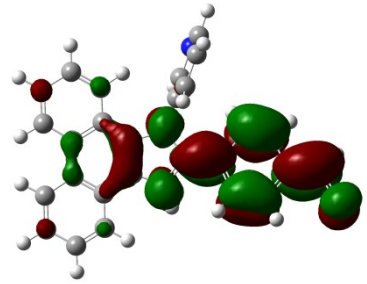
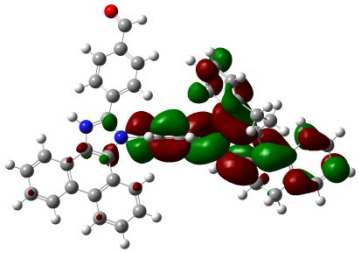
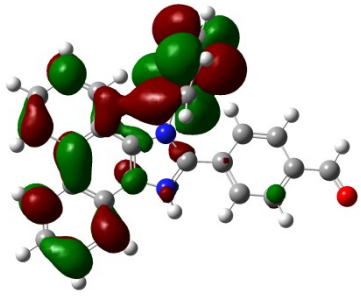
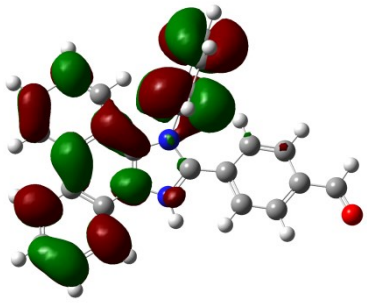



**Figure-S21** Optimized structure of 7, 9a-c, 7+MeOH and 9a+ MeOH

| Entry | λ (nm) | Oscillator Strength, *f* | Energy (eV) | Selected Major Transitions [a] |
|---|---|---|---|---|
| 7 | 652 | 0.0192 | 1.62 | H → L (81%) |
| | 645 | 0.0670 | 1.76 | H → L+2 (55%) |
| | 632 | 0.2123 | 1.96 | H → L+3 (78%) |
| | 566 | 0.0747 | 2.19 | H → L+5 (62%) |
| | 437 | 0.7444 | 2.83 | H-1 → L+1 (79%) |
| | 431 | 0.0102 | 2.88 | H → L+7 (42%), H → L+8 (36%) |
| | 417 | 0.0374 | 2.97 | H → L+9 (52%) |
| 9a | 690 | 0.0902 | 1.80 | H → L+2 (82%) |
| | 609 | 0.2488 | 2.03 | H → L+4 (87%) |
| | 436 | 0.7907 | 2.84 | H-1 → L+1 (83%) |
| 9b | 673 | 0.1723 | 1.84 | H → L+3 (79%) |
| | 595 | 0.1856 | 2.08 | H → L+ 4(89%) |
| | 527 | 0.0251 | 2.35 | H → L+5 (80%) |
| | 437 | 0.8118 | 2.83 | H-1 → L (83%) |
| 9c | 692 | 0.0576 | 1.79 | H → L+1 (40%), H → L+2 (59%) |
| | 636 | 0.1888 | 1.95 | H → L+3 (87%) |
| | 584 | 0.1118 | 2.12 | H → L+4 (89%) |
| | 437 | 0.7972 | 2.83 | H-1 → L (84%) |
| | 335 | 0.0412 | 3.70 | H-4 → L (42%) |
| 9a+MeOH | 434 | 0.5709 | 2.85 | H → L (99%) |
| | 367 | 0.0171 | 3.38 | H-1 → L (97%) |
| | 309 | 0.0771 | 4.01 | H-1 → L+1 (85%) |
| | 306 | 0.0641 | 4.05 | H-2 → L (61%) |
| | 301 | 0.0349 | 4.11 | H-1 → L+1 (69%) |
| | 293 | 0.0204 | 4.22 | H-5 → L (46%) |

**Table-S1** Major transition achieved from TDDFT calculation with B3LYP/6-31G* level of theory

| Orbitals | 7 | 9a | 9b |
|---|---|---|---|
| HOMO-3 | |  |  |
| HOMO-2 |  |  |  |
| HOMO-1 |  |  |  |
| HOMO |  |  |  |
| LUMO |  |  |  |

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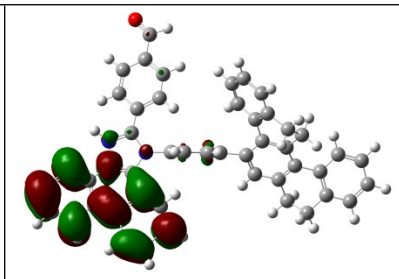
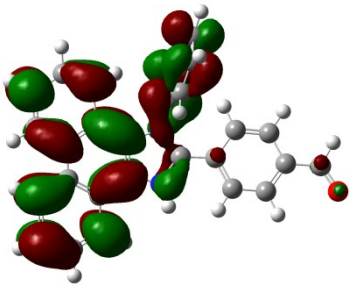
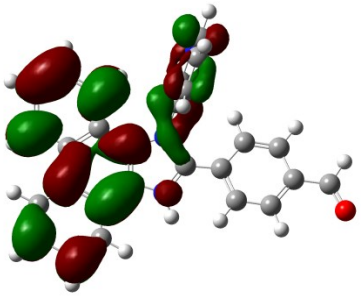
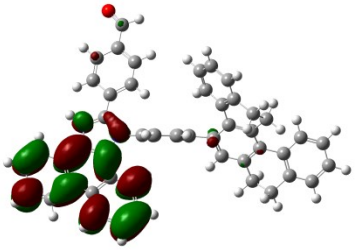
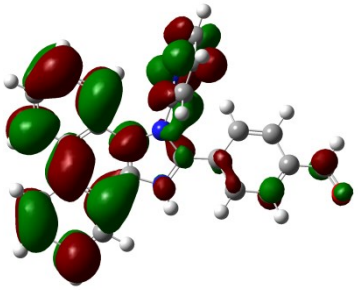
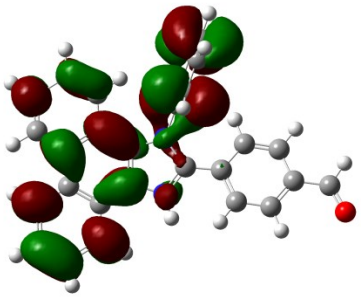
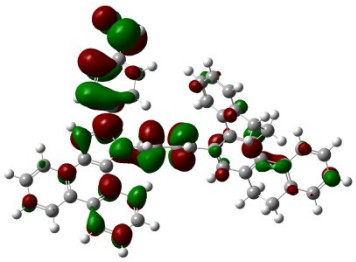
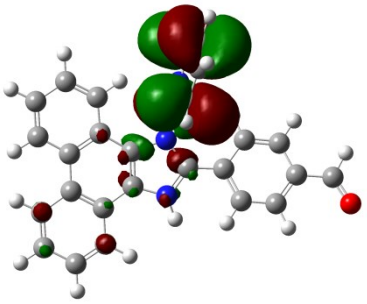
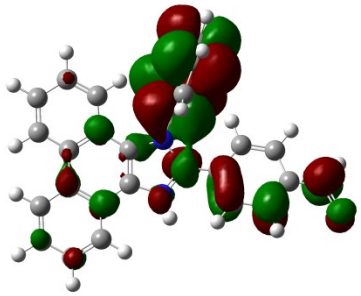
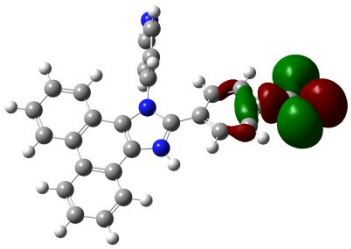
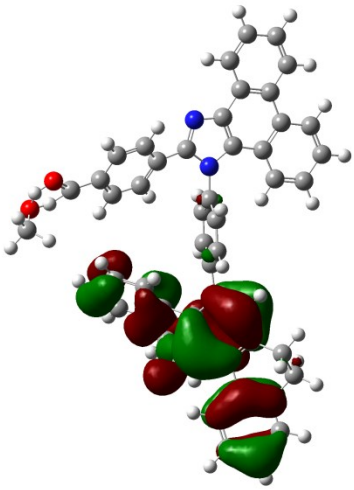
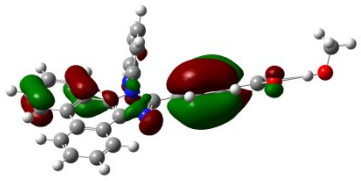
| **LUMO+ 1** |  |  |  |
| **LUMO+ 2** |  |  |  |
| **LUMO+ 3** |  |  |  |

| **Orbitals** | **9c** | **7+MeOH** | **9a+MeOH** |
|---|---|---|---|
| **HOMO-3** |  |  |  |

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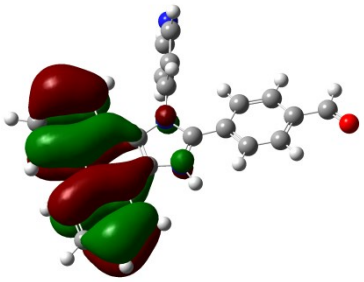
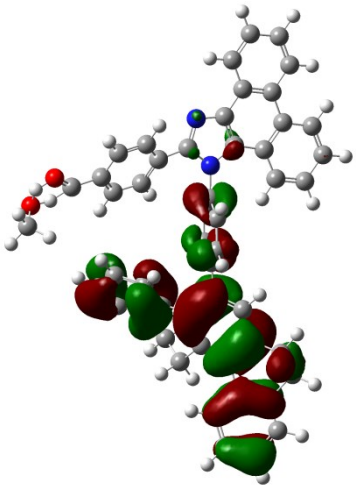
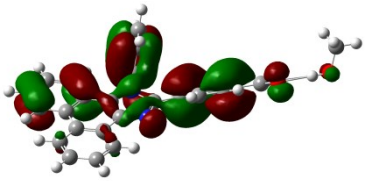
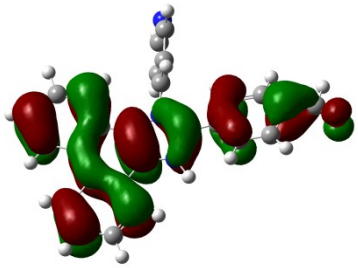
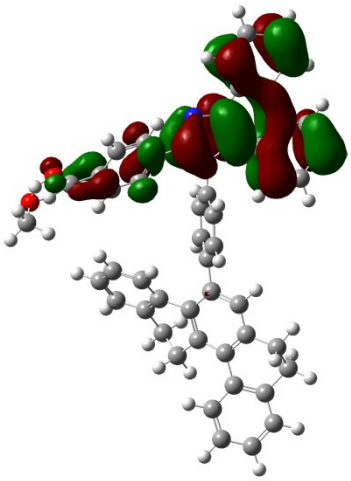
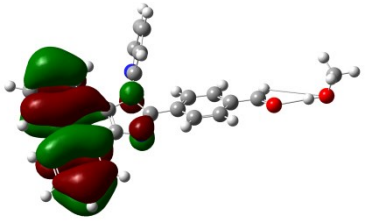
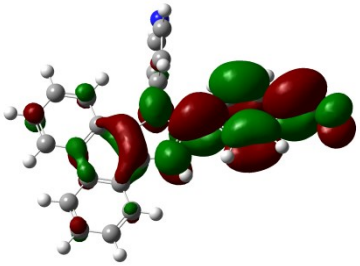
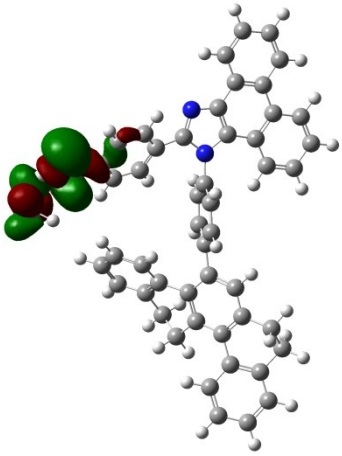
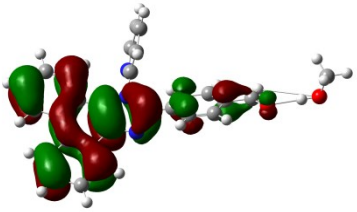
| **HOMO-2** |  |  |  |
| **HOMO-1** |  |  |  |
| **HOMO** |  |  |  |

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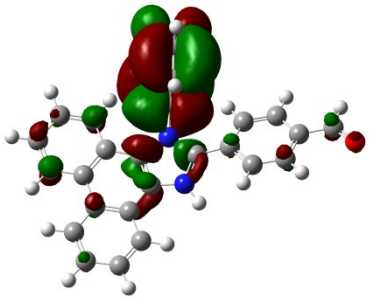
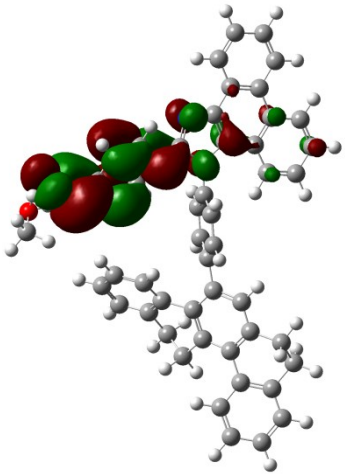
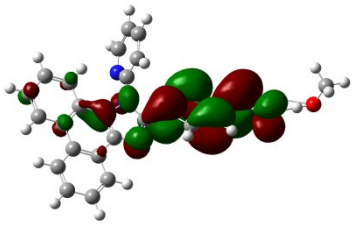
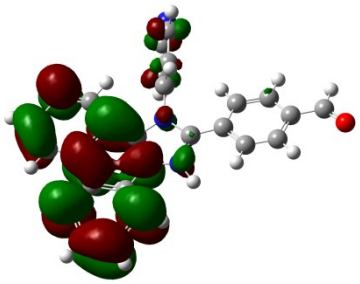
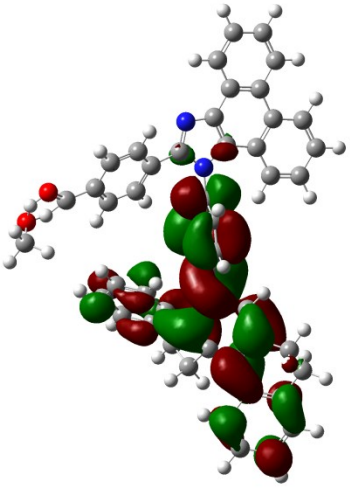
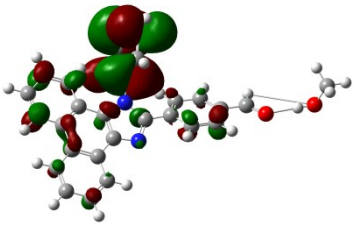
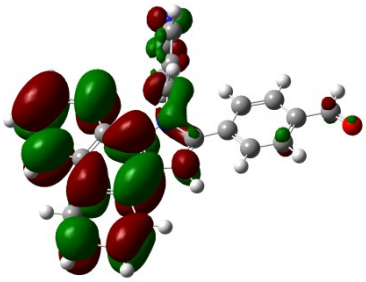
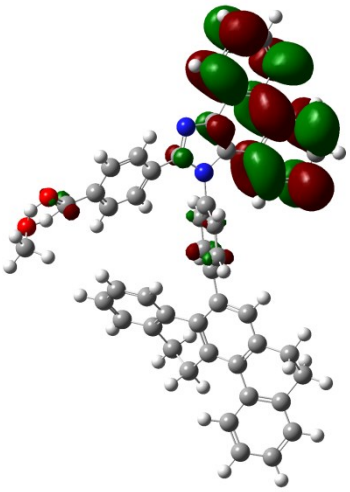
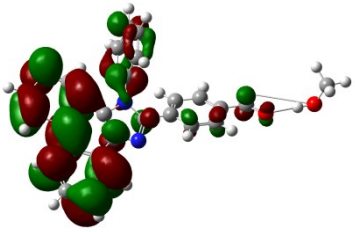
| **LUMO** |  |  |  |
| **LUMO+ 1** |  |  |  |
| **LUMO+ 2** |  |  |  |

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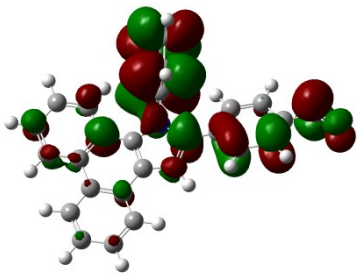
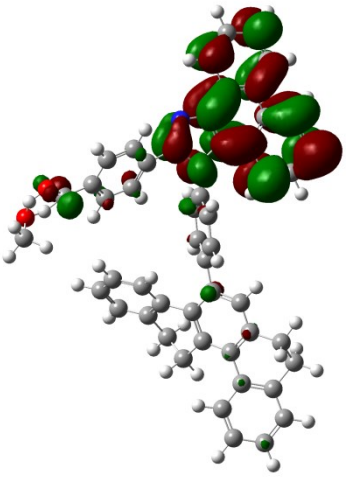
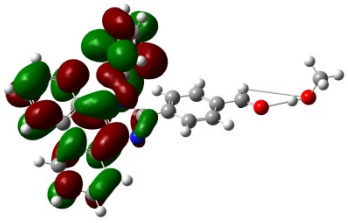
| **LUMO+ 3** |  |  |  |

**Table-S2** Density surfaces of the frontier orbitals involved in electronic transitions of chromophores 7, 9a-c , 7+MeOH and 9a+MeOH which is derived from B3LYP/6-31+G** level of theory.

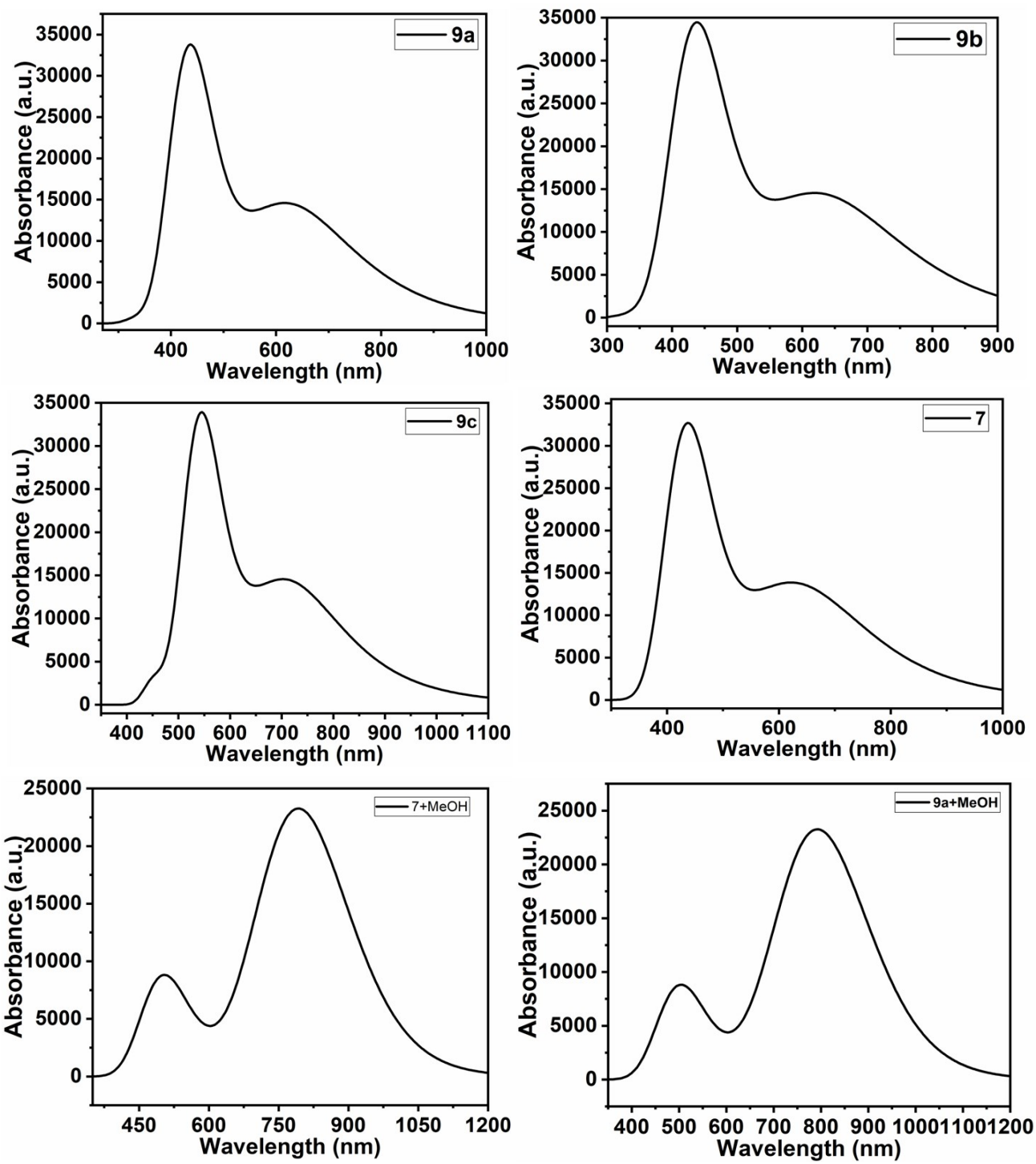



**Figure-S22** Theoretically calculated absorption spectra of fluorophore compound 7, 9a-c, 7+MeOH and 9a+MeOH.

| 7 ( in Acetonitrile solvent medium) | | | | 9a ( in Acetonitrile solvent medium) | | | | 9b (in Acetonitrile solvent medium) | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| C | 9.56746 | -1.85386 | -0.96453 | C | -1.58974 | 4.3799 | -0.49069 | C | -1.52895 | 4.4485 | -0.24502 |
| C | 8.55845 | -2.81319 | -1.09019 | C | -1.44393 | 3.53762 | -1.59338 | C | -1.43284 | 3.68532 | -1.41146 |
| C | 7.21222 | -2.47139 | -0.92768 | C | -0.95898 | 2.24379 | -1.39319 | C | -0.96908 | 2.37387 | -1.31696 |
| C | 6.85649 | -1.13863 | -0.60043 | C | -0.64803 | 1.86182 | -0.0886 | C | -0.62644 | 1.89018 | -0.05406 |
| C | 7.88049 | -0.17579 | -0.52906 | N | -0.78177 | 2.64957 | 0.97955 | C | -0.75945 | 2.72517 | 1.05963 |
| C | 9.2214 | -0.52627 | -0.70243 | C | -1.24416 | 3.89247 | 0.77232 | N | -1.19946 | 3.98622 | 0.97257 |
| C | 6.10654 | -3.47385 | -1.16417 | N | -0.14677 | 0.53269 | 0.15243 | N | -0.14191 | 0.55019 | 0.1099 |
| C | 4.97582 | -2.78406 | -1.94097 | C | 1.21215 | 0.14453 | 0.11632 | C | 1.21369 | 0.14588 | 0.06784 |
| C | 4.48359 | -1.58418 | -1.16225 | C | 1.22834 | -1.23136 | 0.04107 | C | 1.21238 | -1.2314 | 0.02633 |
| C | 5.41289 | -0.80324 | -0.43286 | N | -0.08404 | -1.6645 | 0.01955 | N | -0.10368 | -1.6487 | 0.01751 |
| C | 3.1277 | -1.28601 | -1.09299 | C | -0.94692 | -0.60196 | 0.10072 | C | -0.95788 | -0.57705 | 0.07632 |
| C | 2.63301 | -0.21209 | -0.33768 | C | 2.4294 | 0.90987 | 0.14312 | C | 2.44316 | 0.89438 | 0.06266 |
| C | 3.5495 | 0.58007 | 0.3962 | C | 3.65916 | 0.16683 | 0.08155 | C | 3.66215 | 0.13018 | 0.04077 |
| C | 4.92662 | 0.22364 | 0.41041 | C | 3.65741 | -1.29663 | 0.0046 | C | 3.6396 | -1.33475 | 0.01491 |
| C | 3.14925 | 1.80524 | 1.14722 | C | 2.42229 | -2.01157 | -0.0162 | C | 2.39429 | -2.03081 | -0.00144 |
| C | 3.85208 | 2.13518 | 2.32741 | C | 2.47999 | 2.32309 | 0.2321 | C | 2.51977 | 2.30949 | 0.07523 |
| C | 5.01638 | 1.25606 | 2.70091 | C | 3.68792 | 2.99808 | 0.25148 | C | 3.73856 | 2.96492 | 0.07409 |
| C | 5.81105 | 0.92853 | 1.42792 | C | 4.89449 | 2.28057 | 0.18271 | C | 4.93328 | 2.22553 | 0.05763 |
| C | 2.15424 | 2.68725 | 0.68963 | C | 4.87062 | 0.89817 | 0.10224 | C | 4.88545 | 0.84166 | 0.03988 |
| C | 1.81968 | 3.83218 | 1.41551 | C | 4.8475 | -2.06222 | -0.05389 | C | 4.81817 | -2.11997 | -0.00137 |
| C | 2.48118 | 4.1223 | 2.61247 | C | 4.81996 | -3.44582 | -0.13164 | C | 4.76974 | -3.50465 | -0.03793 |
| C | 3.50363 | 3.27802 | 3.05417 | C | 3.59225 | -4.13502 | -0.15681 | C | 3.53176 | -4.17535 | -0.06175 |
| C | 1.14723 | -0.07474 | -0.27434 | C | 2.40753 | -3.42313 | -0.09965 | C | 2.35785 | -3.44384 | -0.04348 |
| C | 0.46796 | -0.05751 | 0.95815 | C | -2.3607 | -0.72246 | 0.12111 | C | -2.37284 | -0.69805 | 0.08192 |
| C | -0.92405 | -0.03491 | 1.01122 | C | -2.96621 | -1.94861 | -0.3238 | C | -2.96134 | -1.94878 | -0.31997 |
| C | -1.66229 | -0.04051 | -0.17647 | C | -4.32755 | -2.13223 | -0.29345 | C | -4.32013 | -2.14969 | -0.29867 |
| C | -1.01316 | -0.05374 | -1.4113 | C | -5.20354 | -1.11291 | 0.18874 | C | -5.21551 | -1.12383 | 0.1292 |
| C | 0.38226 | -0.06784 | -1.45405 | C | -4.60644 | 0.10069 | 0.63731 | C | -4.63933 | 0.11606 | 0.52783 |
| N | -3.09874 | -0.05957 | -0.12274 | C | -3.24419 | 0.2983 | 0.60747 | C | -3.27928 | 0.33043 | 0.50715 |
| C | -3.90162 | -1.20427 | 0.06997 | C | -6.62826 | -1.28278 | 0.23099 | C | -6.63873 | -1.31167 | 0.16301 |
| C | -5.21305 | -0.78691 | -0.01754 | O | -7.26132 | -2.30277 | -0.13151 | O | -7.25265 | -2.35528 | -0.16006 |
| N | -5.1997 | 0.56622 | -0.28253 | H | -1.96152 | 5.39274 | -0.60045 | H | -1.88559 | 5.47417 | -0.28871 |
| C | -3.91406 | 1.04236 | -0.34395 | H | -1.69774 | 3.87855 | -2.59177 | H | -1.71199 | 4.11105 | -2.3691 |
| C | -3.5713 | -2.58922 | 0.28744 | H | -0.82311 | 1.55181 | -2.21672 | H | -0.87291 | 1.74134 | -2.19344 |
| C | -4.67534 | -3.49388 | 0.46938 | H | -1.34264 | 4.51908 | 1.65443 | H | -0.49759 | 2.35538 | 2.04812 |
| C | -6.06137 | -3.02061 | 0.42139 | H | -0.38056 | -2.62192 | 0.13474 | H | -0.40921 | -2.6014 | 0.14477 |
| C | -6.33929 | -1.64574 | 0.15874 | H | 1.56506 | 2.8927 | 0.29965 | H | 1.61575 | 2.89948 | 0.08261 |
| C | -2.25024 | -3.10267 | 0.31391 | H | 3.69748 | 4.08134 | 0.32245 | H | 3.76479 | 4.05016 | 0.08421 |
| C | -2.0058 | -4.44862 | 0.52413 | H | 5.84525 | 2.80433 | 0.19625 | H | 5.89278 | 2.73321 | 0.05623 |
| C | -3.07818 | -5.33643 | 0.71431 | H | 5.8162 | 0.37246 | 0.05607 | H | 5.82199 | 0.29833 | 0.02326 |
| C | -4.37844 | -4.86105 | 0.68288 | H | 5.81227 | -1.57048 | -0.03989 | H | 5.7903 | -1.64312 | 0.01391 |
| C | -7.17153 | -3.87755 | 0.61931 | H | 5.75318 | -3.99877 | -0.17501 | H | 5.69457 | -4.07304 | -0.0497 |
| C | -8.4743 | -3.40822 | 0.555 | H | 3.57386 | -5.21835 | -0.22146 | H | 3.4972 | -5.25971 | -0.09425 |
| C | -8.73106 | -2.04946 | 0.28818 | H | 1.46224 | -3.95626 | -0.12404 | H | 1.40458 | -3.96295 | -0.06445 |
| C | -7.67317 | -1.17936 | 0.09336 | H | -2.34768 | -2.74113 | -0.73507 | H | -2.33119 | -2.75095 | -0.69231 |
| C | -3.59547 | 2.40352 | -0.60175 | H | -4.75589 | -3.06215 | -0.65444 | H | -4.73096 | -3.09967 | -0.62625 |
| C | -2.32144 | 3.01189 | -0.34317 | H | -5.24615 | 0.88898 | 1.02814 | H | -5.2934 | 0.91491 | 0.87036 |
| C | -2.11239 | 4.35172 | -0.58315 | H | -2.84309 | 1.224 | 0.99806 | H | -2.90311 | 1.28378 | 0.8501 |
| C | -3.13413 | 5.19993 | -1.09928 | H | -7.19091 | -0.41321 | 0.6253 | H | -7.21769 | -0.43316 | 0.51141 |
| C | -4.40108 | 4.59883 | -1.36597 | | | | | | | | |
| C | -4.62267 | 3.26442 | -1.12719 | | | | | | | | |
| C | -2.87828 | 6.59172 | -1.3369 | | | | | | | | |
| O | -3.69782 | 7.42663 | -1.78985 | | | | | | | | |
| H | 10.60803 | -2.13594 | -1.09638 | | | | | | | | |

| | | |
|---|---|---|
| H 8.81637 -3.84054 -1.33531 | | |
| H 7.63318 0.86576 -0.36342 | | |
| H 9.98911 0.23963 -0.64164 | | |
| H 5.71021 -3.84462 -0.20753 | | |
| H 6.49008 -4.33862 -1.71371 | | |
| H 4.14723 -3.47424 -2.12578 | | |
| H 5.35938 -2.46813 -2.92255 | | |
| H 2.42323 -1.93033 -1.61165 | | |
| H 4.66586 0.31976 3.15909 | | |
| H 5.65809 1.75625 3.43253 | | |
| H 6.66487 0.29587 1.67796 | | |
| H 6.21589 1.86606 1.02005 | | |
| H 1.64362 2.48741 -0.24567 | | |
| H 1.04992 4.5008 1.04218 | | |
| H 2.22108 5.00947 3.18261 | | |
| H 4.05076 3.51636 3.96297 | | |
| H 1.03399 -0.07518 1.88346 | | |
| H -1.43885 -0.03056 1.96669 | | |
| H -1.59324 -0.05632 -2.32852 | | |
| H 0.8824 -0.07454 -2.41744 | | |
| H -6.01242 1.16215 -0.30021 | | |
| H -1.4117 -2.43949 0.16313 | | |
| H -0.98319 -4.81299 0.53795 | | |
| H -2.89314 -6.39332 0.87939 | | |
| H -5.18522 -5.57003 0.8215 | | |
| H -7.01694 -4.92863 0.82926 | | |
| H -9.2999 -4.09543 0.71281 | | |
| H -9.75218 -1.68492 0.23777 | | |
| H -7.87476 -0.1315 -0.10758 | | |
| H -1.51172 2.42819 0.0711 | | |
| H -1.13684 4.77983 -0.36478 | | |
| H -1.19589 5.21207 -1.77908 | | |
| H -5.59479 2.85699 -1.38753 | | |
| H -1.85139 6.92685 -1.08941 | | |

| 9c ( in Acetonitrile solvent medium) | 7+MeOH ( in Acetonitrile solvent medium) | 9a+MeOH (in Acetonitrile solvent medium) |
|---|---|---|
| N -1.60665 4.48239 -0.39019 | C 2.9934 0.6121 2.708 | C 0.48349 4.5537 0.1437 |
| C -1.22865 4.03471 0.81762 | C 2.6129 1.2441 1.5112 | C 0.01559 3.97403 -1.03851 |
| C -0.73928 2.74711 1.04533 | C 1.3468 0.9802 0.9349 | N -0.37969 2.69455 -1.12475 |
| C -0.6349 1.88481 -0.04648 | C 0.4895 0.0006 1.5125 | C -0.3219 1.96075 -0.01114 |
| C -1.02202 2.32829 -1.30997 | C 0.8589 -0.5485 2.7661 | C 0.12361 2.43626 1.22215 |
| C -1.50135 3.63568 -1.42558 | C 2.1057 -0.2663 3.3478 | C 0.53884 3.76743 1.29475 |
| N -0.13964 0.54759 0.12529 | C 0.8789 1.7295 -0.2645 | N -0.74824 0.59152 -0.12689 |
| C 1.21842 0.14917 0.08241 | C -0.6616 1.9417 -0.2308 | C -2.05269 0.10159 -0.06032 |
| C 1.22104 -1.22787 0.02693 | C -1.3833 0.6706 0.0801 | C -1.91656 -1.28383 -0.07858 |
| N -0.09333 -1.65002 0.00786 | C -0.7502 -0.3359 0.8582 | N -0.59631 -1.64837 -0.14134 |
| C -0.95112 -0.58187 0.07743 | C -2.6816 0.4574 -0.4277 | C 0.0894 -0.51741 -0.17268 |
| C 2.44605 0.90091 0.07929 | C -3.3907 -0.7437 -0.189 | C -3.33187 0.75522 0.04622 |
| C 3.66713 0.14012 0.05299 | C -2.7386 -1.7702 0.5588 | C -4.48218 -0.10286 0.10908 |
| C 3.6488 -1.32456 0.01817 | C -1.3598 -1.6224 0.9077 | C -4.34479 -1.56681 0.05772 |
| C 2.4054 -2.02356 -0.00669 | C -3.3772 -2.9815 1.0034 | C -3.05351 -2.16181 -0.03272 |
| C 2.5187 2.31601 0.09358 | C -2.6204 -4.1866 1.0317 | C -3.5106 2.15847 0.09605 |
| C 3.73565 2.97483 0.0931 | C -1.2054 -4.1293 0.5888 | C -4.77225 2.719 0.20916 |
| C 4.93246 2.23894 0.07516 | C -0.5652 -2.8632 1.2181 | C -5.90227 1.88796 0.27578 |
| C 4.88844 0.85501 0.05384 | C -4.69 -2.9975 1.5342 | C -5.75124 0.51073 0.22569 |
| C 4.82948 -2.1066 -0.00106 | C -5.2517 -4.1881 2.0283 | C -5.46007 -2.43891 0.09617 |
| C 4.78457 -3.49103 -0.0491 | C -4.499 -5.3748 2.0384 | C -5.3066 -3.81708 0.05259 |
| C 3.54838 -4.16459 -0.08254 | C -3.1845 -5.3765 1.5418 | C -4.02307 -4.38851 -0.03197 |

| | | | |
|---|---|---|---|
| C | 2.37261 | -3.43624 | -0.06117 |
| C | -2.36544 | -0.70592 | 0.08995 |
| C | -2.95512 | -1.94842 | -0.3339 |
| C | -4.31375 | -2.15036 | -0.30647 |
| C | -5.20567 | -1.13448 | 0.151 |
| C | -4.62746 | 0.09682 | 0.57259 |
| C | -3.26777 | 0.31283 | 0.54526 |
| C | -6.6288 | -1.32384 | 0.1916 |
| O | -7.24449 | -2.36023 | -0.14967 |
| H | -1.32233 | 4.73329 | 1.6447 |
| H | -0.45081 | 2.42735 | 2.04056 |
| H | -0.95293 | 1.6807 | -2.17694 |
| H | -1.81063 | 4.0159 | -2.39555 |
| H | -0.39628 | -2.60408 | 0.1317 |
| H | 1.61317 | 2.90351 | 0.10424 |
| H | 3.75876 | 4.06015 | 0.10467 |
| H | 5.89055 | 2.74928 | 0.07458 |
| H | 5.8265 | 0.31436 | 0.03456 |
| H | 5.80043 | -1.62759 | 0.02109 |
| H | 5.71087 | -4.05699 | -0.0627 |
| H | 3.51665 | -5.24873 | -0.12451 |
| H | 1.42076 | -3.95758 | -0.08913 |
| H | -2.32628 | -2.74095 | -0.72867 |
| H | -4.72715 | -3.09307 | -0.65147 |
| H | -5.27949 | 0.88665 | 0.93916 |
| H | -2.88784 | 1.25805 | 0.90711 |
| H | -7.20544 | -0.45354 | 0.56367 |

| | | | |
|---|---|---|---|
| C | -4.6909 | -0.8892 | -0.7821 |
| C | -5.0211 | -2.0272 | -1.5617 |
| C | -6.2886 | -2.1573 | -2.1612 |
| C | -7.2547 | -1.1374 | -2.0242 |
| C | -6.9393 | -0.0031 | -1.2459 |
| C | -5.681 | 0.1128 | -0.6266 |
| N | -8.486 | -1.2538 | -2.6164 |
| C | -8.8051 | -1.1745 | -3.939 |
| C | -10.1784 | -1.3964 | -4.0146 |
| N | -10.6738 | -1.5443 | -2.7793 |
| C | -9.6406 | -1.456 | -1.9278 |
| C | -8.0669 | -0.9131 | -5.1267 |
| C | -8.7472 | -0.9563 | -6.3954 |
| C | -10.1587 | -1.2202 | -6.4485 |
| C | -10.8788 | -1.4397 | -5.2327 |
| C | -6.688 | -0.5837 | -5.0962 |
| C | -5.9566 | -0.362 | -6.2689 |
| C | -6.6 | -0.4279 | -7.5071 |
| C | -7.9714 | -0.7184 | -7.5667 |
| C | -10.9158 | -1.2692 | -7.6555 |
| C | -12.2957 | -1.538 | -7.6613 |
| C | -12.9726 | -1.7553 | -6.454 |
| C | -12.2695 | -1.6994 | -5.2422 |
| C | -9.8131 | -1.5465 | -0.5239 |
| C | -9.0064 | -2.4045 | 0.2578 |
| C | -9.1292 | -2.4247 | 1.659 |
| C | -10.0704 | -1.5963 | 2.3038 |
| C | -10.9072 | -0.7689 | 1.5249 |
| C | -10.7863 | -0.7511 | 0.123 |
| C | -10.1581 | -1.6011 | 3.707 |
| H | -9.6563 | -2.0907 | 4.4309 |
| O | -10.8512 | -0.9778 | 4.5537 |
| O | -9.703 | -2.0779 | 5.3922 |
| H | -10.4102 | -1.4074 | 5.214 |
| C | -8.685 | -2.1564 | 6.3941 |
| H | 3.9095 | 0.8003 | 3.1211 |
| H | 3.2628 | 1.8988 | 1.0675 |
| H | 0.2173 | -1.146 | 3.2856 |
| H | 2.3653 | -0.6999 | 4.2374 |
| H | 1.3625 | 2.7083 | -0.3353 |
| H | 1.1391 | 1.1539 | -1.1563 |
| H | -0.9181 | 2.6875 | 0.5266 |
| H | -0.9659 | 2.3361 | -1.2061 |
| H | -3.1113 | 1.2001 | -0.9863 |
| H | -0.6444 | -5.0185 | 0.8873 |
| H | -1.1736 | -4.0569 | -0.5025 |
| H | -0.5 | -3.0183 | 2.2956 |
| H | 0.4471 | -2.7745 | 0.8153 |
| H | -5.2385 | -2.1379 | 1.5958 |
| H | -6.2039 | -4.1883 | 2.397 |
| H | -4.9011 | -6.234 | 2.4217 |
| H | -2.6368 | -6.241 | 1.5682 |
| H | -4.338 | -2.7745 | -1.7079 |
| H | -6.504 | -2.9948 | -2.7076 |
| H | -7.6263 | 0.7464 | -1.1284 |
| H | -5.4927 | 0.9439 | -0.06 |
| H | -6.178 | -0.473 | -4.2276 |
| H | -4.9582 | -0.1455 | -6.2164 |
| H | -6.0699 | -0.2573 | -8.3652 |
| H | -8.3758 | -0.7459 | -8.4999 |

| | | | |
|---|---|---|---|
| C | -2.90999 | -3.56532 | -0.07481 |
| C | 1.55783 | -0.47706 | -0.25116 |
| C | 2.25819 | 0.49427 | -0.99002 |
| C | 3.64852 | 0.45535 | -1.05366 |
| C | 4.366 | -0.55064 | -0.38672 |
| C | 3.66743 | -1.53191 | 0.34212 |
| C | 2.28265 | -1.49562 | 0.40635 |
| C | 5.83097 | -0.55826 | -0.47092 |
| H | 6.27831 | 0.24922 | -1.08122 |
| O | 6.5575 | -1.38476 | 0.08075 |
| H | 8.40713 | -1.26472 | -0.09272 |
| O | 9.36745 | -1.1214 | -0.20213 |
| C | 9.89526 | -0.62407 | 1.02689 |
| H | 0.7941 | 5.59271 | 0.15498 |
| H | -0.04171 | 4.55444 | -1.95535 |
| H | 0.13849 | 1.78552 | 2.0891 |
| H | 0.89418 | 4.17917 | 2.23372 |
| H | -2.65234 | 2.81289 | 0.04059 |
| H | -4.88156 | 3.79859 | 0.24521 |
| H | -6.89466 | 2.31877 | 0.36703 |
| H | -6.64197 | -0.10282 | 0.28197 |
| H | -6.46475 | -2.03868 | 0.15863 |
| H | -6.18491 | -4.45491 | 0.08314 |
| H | -3.90654 | -5.46764 | -0.06565 |
| H | -1.91136 | -3.98431 | -0.14324 |
| H | 1.722 | 1.26047 | -1.536 |
| H | 4.18171 | 1.20408 | -1.63321 |
| H | 4.22309 | -2.30985 | 0.85527 |
| H | 1.74054 | -2.24677 | 0.96954 |
| H | 10.95988 | -0.43022 | 0.872 |
| H | 9.41165 | 0.31449 | 1.32916 |
| H | 9.78975 | -1.35299 | 1.84175 |

| | | |
|---|---|---|
| | H -10.4913 -1.1119 -8.567<br>H -12.8088 -1.5791 -8.5469<br>H -13.9755 -1.9552 -6.4563<br>H -12.7845 -1.8502 -4.3703<br>H -8.3235 -3.0251 -0.1842<br>H -8.524 -3.046 2.2013<br>H -11.6048 -0.168 1.9708<br>H -11.4034 -0.1382 -0.4174<br>H -9.1401 -2.1499 7.3855<br>H -8.0067 -1.3069 6.3022<br>H -8.123 -3.0812 6.2603 | |

**Table S3** Cartesian coordinates (in Angstroms) of the optimized geometries in ground state of 7, 9a-c, 7+MeOH and 9a+MeOH in acetonitrile solvent method at B3LYP/6-31+G** level

| S.No | Reported Probe | Analytical | LOD | Applications | Reference |
|---|---|---|---|---|---|

| | | **methods** | | | |
|---|---|---|---|---|---|
| 1 | N,bis(5-nitro-salicylaldehyde)azine | UV, FL | - | DNA studies | New J. Chem., 2019, 43, 8982--8992 |
| 2 | carboxen–polydimethylsiloxane | GC | - | Biodiesel | Bioresource Technology 99 (2008) 5901–5905 |
| 3 | (E)-4-((4-(dimethylamino)benzylidene)amino)benzonitrile | UV, FL | 9.65ppm | - | Sensors and Actuators B: Chemical, 2020, 319, 128323. |
| 4 | Pentacenequinone derivative | UV, FL | 0.038% | - | Chemical Communications, 2018, 54(60), 8339-8342. |
| 5 | Oxoporphyrinogen-LDH | UV | - | - | ACS Appl. Mater. Interfaces 2013, 5, 5927−5930 |
| 6 | Ln-CPs | PL | - | - | RSC Advances, 2014 4(27), 14035-14041. |
| 7 | (3-(((7-(diethylamino)-2-oxo-2H-chromen-3yl)methylene)amino)-2-thioxothiazolidin-4-one | UV,FL | Upto 5% | Bio-Imaging | Organic & biomolecular chemistry, 2015, 13(33), 8822-8826. |
| **8** | **Imidazole based** | **UV,FL** | **9 to 10ppm** | **Biodiesel, Paper strip** | **Present work** |

**Table S4** Comparison table of imidazole-based probe for detection of methanol in previous and present reports