

Supporting information

Design, synthesis and electronic properties of push-pull-push type dye

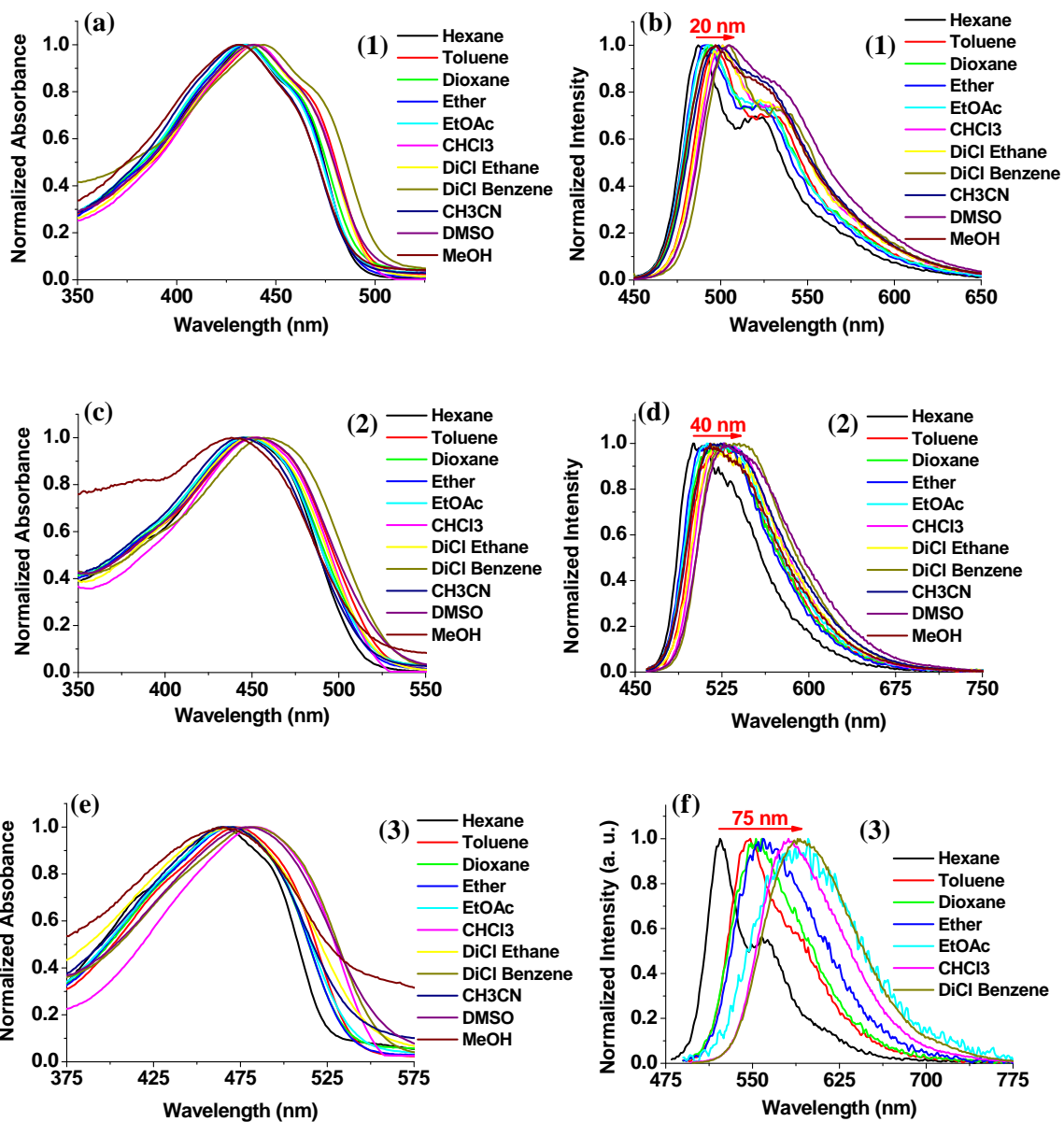
Rajen Kundu,*^a Chandramouli Kulshreshtha *^b

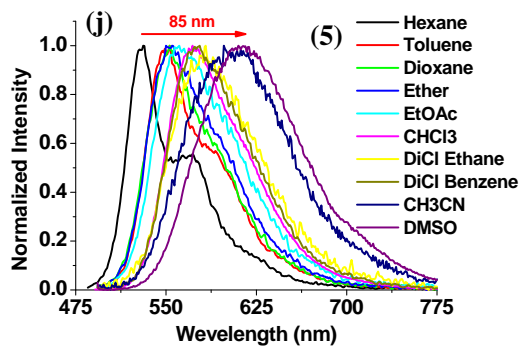
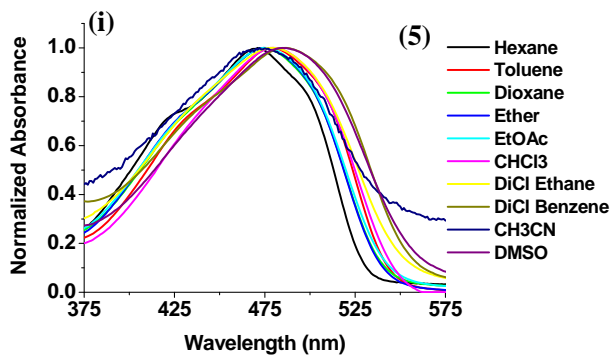
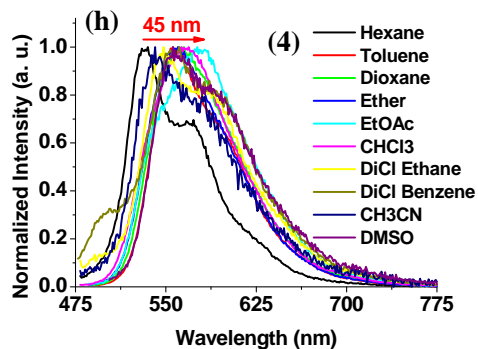
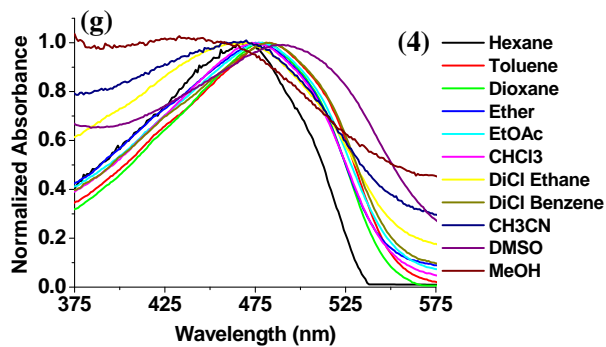
^a Department of Chemistry, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

^b Department of Chemical Engineering, Pohang University of Science and Technology, Pohang 790-784, Republic of Korea

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1. Normalized UV-visible and fluorescence spectra of the dyes (1 – 5)





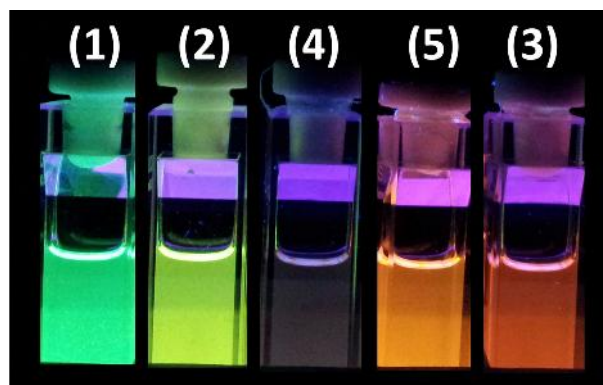
2. Photophysical data of the dyes (1 – 5)

1				2			
Solvents	Max ^{Abs} (nm)	(M ⁻¹ cm ⁻¹)	Max ^{Fl} (nm)	Solvents	Max ^{Abs} (nm)	(M ⁻¹ cm ⁻¹)	Max ^{Fl} (nm)
Hexane	437	45000	487	Hexane	450	30200	500
Toluene	441	43700	497	Toluene	454	42700	527
Dioxane	436	47900	495	Dioxane	449	40500	525
Ether	437	43700	492	Ether	450	39100	523
EtOAc	435	47200	493	EtOAc	451	40500	525
CHCl ₃	440	45400	501	CHCl ₃	453	37100	529
DiClEthane	439	45600	501	DiClEthane	452	37800	526
DiClBenzene	446	45400	504	DiClBenzene	463	35600	540
CH ₃ CN	433	42600	500	CH ₃ CN	447	37700	527
DMSO	440	44700	507	DMSO	456	37200	532
MeOH	432	30200	498	MeOH	445	13000	522

3				4			
Solvents	Max ^{Abs} (nm)	(M ⁻¹ cm ⁻¹)	Max ^{Fl} (nm)	Solvents	Max ^{Abs} (nm)	(M ⁻¹ cm ⁻¹)	Max ^{Fl} (nm)
Hexane	465	19700	520	Hexane	473	7700	533
Toluene	473	37100	548	Toluene	483	19800	557
Dioxane	470	36200	555	Dioxane	478	20700	564
Ether	470	35000	562	Ether	477	22400	559
EtOAc	471	34700	595	EtOAc	480	20800	578
CHCl ₃	485	30600	581	CHCl ₃	477	18000	566
DiClEthane	470	26900	603	DiClEthane	472	15000	550
DiClBenzene	485	30500	593	DiClBenzene	482	25700	559
CH ₃ CN	470	27500		CH ₃ CN	475	6300	545
DMSO	481	31500		DMSO	494	15300	560
MeOH	466	11100		MeOH	470	5000	

5			
Solvents	Max ^{Abs} (nm)	(M ⁻¹ cm ⁻¹)	Max ^{Fl} (nm)
Hexane	471	28100	530
Toluene	478	67700	551
Dioxane	475	66400	553
Ether	476	68600	554
EtOAc	475	69000	560
CHCl ₃	482	62500	572
DiClEthane	480	57500	582
DiClBenzene	488	63800	577
CH ₃ CN	472	6100	609
DMSO	487	45700	615
MeOH	472	3700	

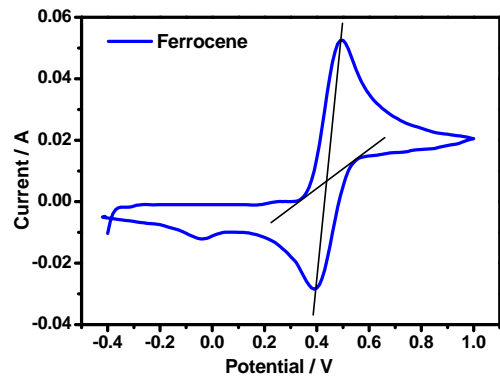
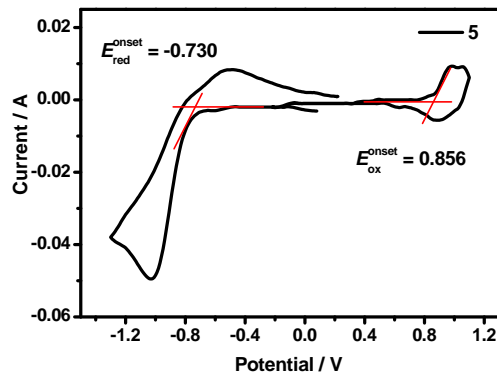
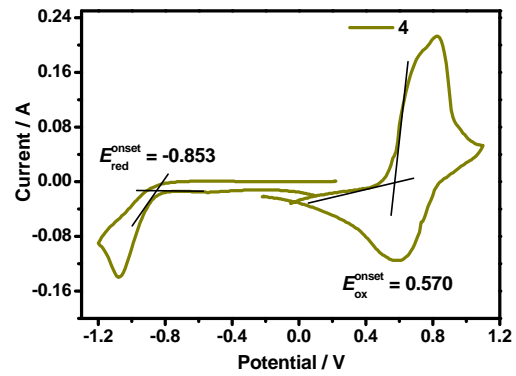
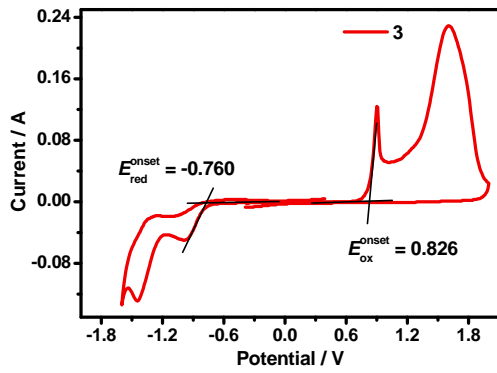
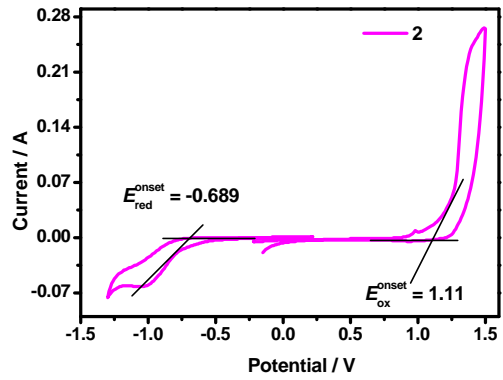
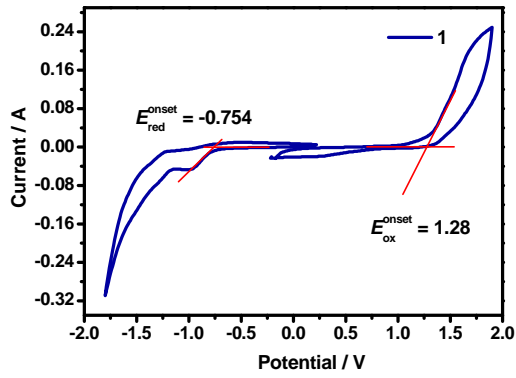
3. Colour of the fluorescence images of the dyes (1 – 5) in *o*-Dichlorobenzene under a 254 nm wavelength transilluminator



4. Colour of the fluorescence images and solvatochromism of the dyes (1 – 5) in different solvents under a 254 nm wavelength transilluminator

Dye	Solvents: Hexane		Toluene		<i>o</i> -Dichlorobenzene		CHCl ₃	
	EtOAc	DMSO	CH ₃ CN	MeOH	MeOH	MeOH	MeOH	MeOH
1								
2								
3								
4								
5								

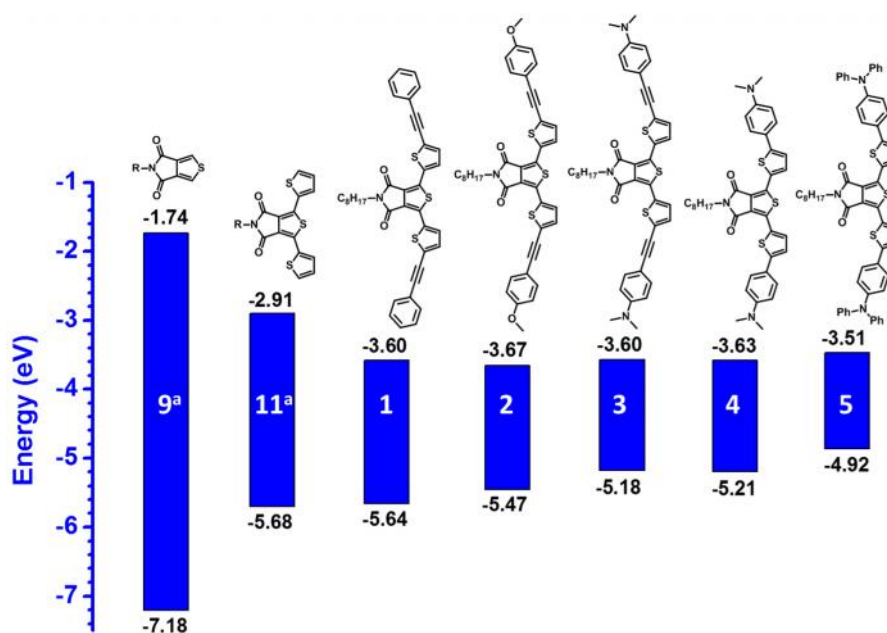
5. Cyclic voltammetry diagram of dyes 1-5, representing E_{ox} and E_{red}



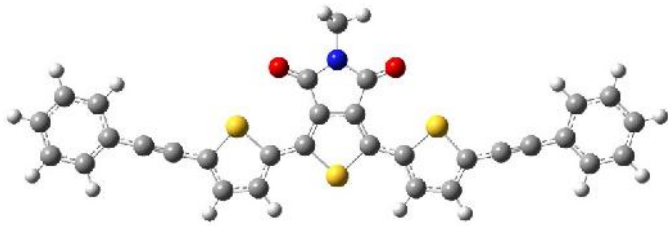
6. Energy parameters of the dyes 1–5

Entry	E_{HOMO} (eV)	E_{LUMO} (eV)	$E_{\text{ox-red}}$ (eV)
9^a	(-7.30)	(-1.78)	5.52
11^a	-5.68	-2.91	2.77
1	-5.643	-3.609	2.034
2	-5.473	-3.674	1.799
3	-5.189	-3.603	1.586
4	-5.219	-3.633	1.586
5	-4.929	-3.51	1.419

^a The data were taken from the reference (K. Takimiya, I. Osaka, and M. Nakano, *Chem. Mater.*, 2014, **26**, 587).



7. Cartesian coordinates of the optimized geometry

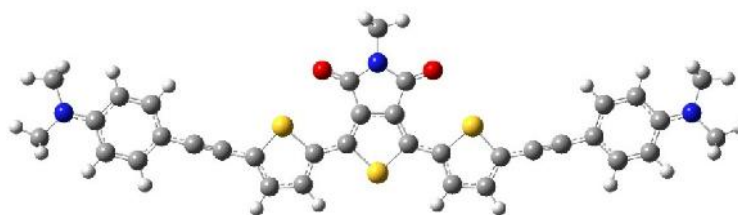
1							
							
O 1				H	-0.50575600	4.70460500	0.89064500
C	-1.29315200	-0.55993800	0.00001600	H	1.04750300	4.63231800	0.00027800
C	-0.71212300	0.68486500	-0.00002400	C	6.54645500	-0.83034700	0.00083900
C	0.70952200	0.68578400	0.00015300	C	7.73507100	-0.57467100	0.00092400
C	1.29280100	-0.55844500	0.00031300	C	-6.54639500	-0.83339500	-0.00084300
C	-1.18412600	2.08164300	-0.00021700	C	-7.73479600	-0.57672700	-0.00111400
O	-2.32866100	2.54749000	-0.00025600	C	9.12143400	-0.26471100	0.00110000
C	1.17978600	2.08205200	0.00011800	C	10.08876900	-1.29196200	0.00132200
O	2.32529200	2.54717100	0.00033000	C	9.55037000	1.07980800	0.00105400
N	-0.00374200	2.85878200	0.00001500	C	11.44512700	-0.97765900	0.00149400
S	0.00071200	-1.77904700	0.00025600	H	9.76190800	-2.32428100	0.00135600
C	2.67147200	-0.95723100	0.00051500	C	10.90931500	1.38190700	0.00122800
C	3.15200000	-2.26334200	0.00070100	H	8.80959700	1.86951700	0.00088200
S	3.99986500	0.19216600	0.00061700	C	11.86064900	0.35727900	0.00144700
C	4.55711300	-2.35170400	0.00084400	H	12.18024400	-1.77392200	0.00166500
H	2.50133100	-3.12770400	0.00071000	H	11.22837500	2.41757300	0.00119000
C	5.17435100	-1.10672000	0.00075900	C	-9.12081100	-0.26517900	-0.00149600
H	5.11085500	-3.27869500	0.00097400	C	-10.08942600	-1.29121300	-0.00175000
C	-2.67156000	-0.95980000	-0.00010700	C	-9.54809200	1.07987600	-0.00162900
C	-3.15165200	-2.26598200	-0.00005000	C	-11.44539900	-0.97523200	-0.00212700
S	-4.00009300	0.18947900	-0.00024300	H	-9.76384400	-2.32393700	-0.00164800
C	-4.55682900	-2.35464500	-0.00028400	C	-10.90666200	1.38365800	-0.00200700
H	-2.50075700	-3.13018900	0.00010200	H	-8.80633100	1.86865900	-0.00143300
C	-5.17427200	-1.10980000	-0.00054100	C	-11.85927300	0.36021700	-0.00225700
H	-5.11036100	-3.28176900	-0.00032400	H	-12.18150400	-1.77058500	-0.00232100
C	0.00072500	4.32243900	0.00009100	H	-11.22442900	2.41972500	-0.00210700
H	-0.50546100	4.70469100	-0.89059300	H	12.91732400	0.59723200	0.00158100
				H	-12.91565000	0.60148700	-0.00255000

2



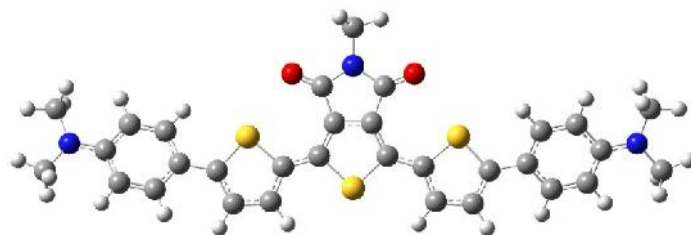
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C	1.29393900	-0.57880500	-0.00001200	C	-9.12025600	-0.28406100	-0.00108900
C	0.71255900	0.66600500	-0.00004900	C	-10.09421500	-1.30031400	-0.00185800
C	-0.70957700	0.66709100	-0.00019100	C	-9.55635000	1.06235000	-0.00063600
C	-1.29351200	-0.57701300	-0.00027500	C	-11.45166800	-0.99182100	-0.00218100
C	1.18471800	2.06214800	0.00003600	H	-9.77621300	-2.33546600	-0.00221100
O	2.32909600	2.52898300	0.00013700	C	-10.90555600	1.36624100	-0.00095100
C	-1.17966500	2.06281300	-0.00019300	H	-8.81918600	1.85520700	-0.00004100
O	-2.32490300	2.52921900	-0.00026800	C	-11.86979300	0.34399900	-0.00173100
N	0.00421400	2.83956000	-0.00005900	H	-12.17375200	-1.79676900	-0.00278800
S	-0.00081900	-1.79810600	-0.00023400	H	-11.25333700	2.39060500	-0.00061700
C	-2.67132500	-0.97617300	-0.00042500	C	9.11966900	-0.28612700	0.00131000
C	-3.15209700	-2.28217400	-0.00062500	C	10.09493900	-1.30110200	0.00189200
S	-4.00142900	0.17282200	-0.00042200	C	9.55402600	1.06085300	0.00113800
C	-4.55701900	-2.37146800	-0.00073100	C	11.45200700	-0.99084900	0.00230000
H	-2.50096200	-3.14626900	-0.00068800	H	9.77827800	-2.33666600	0.00202900
C	-5.17595600	-1.12678900	-0.00060700	C	10.90284200	1.36649300	0.00154100
H	-5.10997000	-3.29893600	-0.00087800	H	8.81582400	1.85274400	0.00069100
C	2.67140000	-0.97938100	0.00015300	C	11.86839200	0.34550700	0.00212800
C	3.15142200	-2.28556500	0.00023100	H	12.17514900	-1.79485400	0.00275200
S	4.00191300	0.16917600	0.00025800	H	11.24928900	2.39131200	0.00142000
C	4.55639500	-2.37549500	0.00042100	C	14.23461300	-0.25132000	0.00327600
H	2.49985600	-3.14935100	0.00017400	H	14.18396100	-0.88345900	-0.89118200
C	5.17582400	-1.13110700	0.00049500	H	15.16778600	0.31173800	0.00353800
H	5.10891300	-3.30323000	0.00052000	H	14.18313300	-0.88293000	0.89806100
C	-0.00023700	4.30287500	-0.00002000	C	-14.23527700	-0.25585300	-0.00301300
H	0.50595500	4.68540700	0.89061000	H	-15.16913200	0.30606700	-0.00316300
H	0.50620900	4.68545100	-0.89048600	H	-14.18300000	-0.88718400	-0.89794400
H	-1.04712500	4.61251800	-0.00015900	H	-14.18385100	-0.88811300	0.89131100
C	-6.54756600	-0.85089800	-0.00067100	O	13.18385900	0.76404500	0.00249300
C	-7.73670900	-0.59476700	-0.00079300	O	-13.18575800	0.76082500	-0.00199200
C	6.54751600	-0.85545100	0.00069400				

3



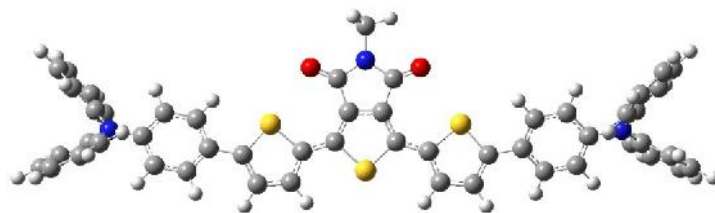
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C	-1.29514800	-0.70485700	0.00007300	H	9.80591700	-2.42997800	0.00795500
C	-0.71314200	0.54011000	-0.00002500	C	10.88708900	1.28460600	-0.00550500
C	0.70978900	0.54127100	-0.00046600	H	8.79834400	1.74472800	-0.01050900
C	1.29450400	-0.70294100	-0.00065400	C	11.89093300	0.28222800	0.00017400
C	-1.18538900	1.93529000	0.00021700	H	12.18090100	-1.86843700	0.00944400
O	-2.32924500	2.40444100	0.00067500	H	11.16736500	2.32842100	-0.00931000
C	1.17981100	1.93603500	-0.00058900	C	-9.11395900	-0.39062100	0.00137500
O	2.32447900	2.40492300	-0.00099100	C	-10.10934500	-1.39102900	-0.00335100
N	-0.00456700	2.71293300	-0.00015600	C	-9.54001400	0.95530600	0.00573100
S	0.00077700	-1.92453800	-0.00029700	C	-11.45557300	-1.06702100	-0.00384900
C	2.67103800	-1.10247400	-0.00093000	H	-9.80829900	-2.43167800	-0.00676400
C	3.15272900	-2.40842000	-0.00061700	C	-10.88436900	1.28438300	0.00532000
S	4.00306100	0.04619800	-0.00157500	H	-8.79496900	1.74161800	0.00941900
C	4.55724100	-2.49861600	-0.00093600	C	-11.88958100	0.28339900	0.00046700
H	2.50117900	-3.27232800	-0.00016300	H	-12.18253500	-1.86686400	-0.00770800
C	5.17839700	-1.25407600	-0.00150000	H	-11.16319000	2.32859100	0.00873400
H	5.10959400	-3.42645100	-0.00078500	N	13.23105700	0.60695200	0.00111100
C	-2.67129700	-1.10597400	0.00035000	N	-13.22929200	0.61000500	-0.00011700
C	-3.15208500	-2.41214900	0.00003000	C	-13.64612200	2.01946800	0.00402300
S	-4.00384500	0.04211400	0.00109200	H	-13.27878900	2.55105900	-0.88400300
C	-4.55665200	-2.50313500	0.00040300	H	-14.73639400	2.06187900	0.00310800
H	-2.50001400	-3.27567900	-0.00046600	H	-13.28054300	2.54516700	0.89624900
C	-5.17842300	-1.25895900	0.00101600	C	-14.24952100	-0.44751000	-0.00644600
H	-5.10846600	-3.43129800	0.00025400	H	-14.17079600	-1.08948600	0.88121500
C	0.00006900	4.17557700	-0.00008800	H	-15.23624900	0.01833700	-0.00614000
H	-0.50636100	4.55888900	-0.89038200	H	-14.16767100	-1.08185200	-0.89930700
H	-0.50591800	4.55879400	0.89049900	C	14.24984300	-0.45198400	0.00853900
H	1.04722400	4.48455800	-0.00033700	H	15.23720800	0.01251100	0.00855900
C	6.54839500	-0.97648300	-0.00176700	H	14.16659300	-1.08574000	0.90167800
C	7.73696900	-0.71261600	-0.00173400	H	14.17072500	-1.09428600	-0.87884600
C	-6.54853700	-0.98170900	0.00139800	C	13.64987500	2.01584000	-0.00355100
C	-7.73690700	-0.71696500	0.00152200	H	14.74020200	2.05671400	-0.00231800
C	9.11438400	-0.38795500	-0.00135600	H	13.28531400	2.54161100	-0.89614400
C	10.10840200	-1.38974900	0.00415600	H	13.28301300	2.54835300	0.88411400
C	9.54229100	0.95738200	-0.00620900				

4



0 1				C	8.50139700	0.75678200	0.45371100
C	-1.29597000	-0.44204700	0.00244000	H	6.46257100	1.26628400	0.81283400
C	-0.71373900	0.80248500	0.00155300	C	9.43495900	-0.21412600	0.01413700
C	0.71148800	0.80321900	-0.00253900	H	9.57425500	-2.22261400	-0.79431100
C	1.29572300	-0.44091800	-0.00308700	H	8.84792100	1.71574800	0.81221600
C	-1.18529600	2.19704800	0.00334700	C	-6.61780600	-0.72985300	-0.00195400
O	-2.32786200	2.67030700	0.00825700	C	-7.54437900	-1.69453100	0.43987500
C	1.18168300	2.19703400	-0.00486000	C	-7.13891500	0.50133600	-0.44522300
O	2.32540700	2.66926400	-0.00972100	C	-8.90844600	-1.45137400	0.43439700
N	-0.00340000	2.97408700	-0.00093300	H	-7.18381000	-2.64404000	0.81819500
S	0.00061600	-1.66202000	-0.00018800	C	-8.50072800	0.75711600	-0.45165600
C	2.66985400	-0.84739800	-0.00589700	H	-6.46171400	1.26612900	-0.81034500
C	3.14855700	-2.15164200	0.00310600	C	-9.43466900	-0.21383300	-0.01310300
S	4.01134400	0.29326900	-0.02669500	H	-9.57485300	-2.22308800	0.79323800
C	4.55652700	-2.24037600	0.00534500	H	-8.84680600	1.71665900	-0.80906200
H	2.49677700	-3.01538800	0.02170200	N	10.79313600	0.03378500	0.02080800
C	5.18335300	-1.00321600	-0.00461000	N	-10.79275800	0.03479100	-0.01925500
H	5.09502100	-3.17629400	0.04561600	C	11.30353200	1.33455400	0.47422200
C	-2.66995400	-0.84927700	0.00532400	H	10.91849800	2.15727800	-0.14334900
C	-3.14864000	-2.15341500	-0.00389700	H	11.03118400	1.53269400	1.51972600
S	-4.01116200	0.29171100	0.02664200	H	12.39214500	1.32907700	0.39898700
C	-4.55673300	-2.24195900	-0.00598400	C	11.73424200	-0.99513100	-0.44037000
H	-2.49693800	-3.01722900	-0.02284500	H	12.75028100	-0.60926700	-0.34279300
C	-5.18332600	-1.00472800	0.00442000	H	11.65476400	-1.91171500	0.15951500
H	-5.09533300	-3.17781800	-0.04642300	H	11.56434900	-1.25724100	-1.49368600
C	0.00179300	4.43608400	-0.00119700	C	-11.73438300	-0.99456900	0.43966600
H	-0.50705500	4.82016200	-0.88992500	H	-11.65408800	-1.91048900	-0.16112600
H	-0.50133900	4.82042000	0.89066400	H	-11.56594300	-1.25793100	1.49293400
H	1.04926600	4.74416800	-0.00480300	H	-12.75033300	-0.60869300	0.34112300
C	6.61786700	-0.72879000	0.00206800	C	-11.30237500	1.33683500	-0.46989700
C	7.54402000	-1.69340800	-0.44076000	H	-10.91531800	2.15810500	0.14832100
C	7.13948500	0.50166700	0.44681700	H	-11.03149500	1.53631900	-1.51554000
C	8.90818700	-1.45091100	-0.43483800	H	-12.39086500	1.33256300	-0.39281500
H	7.18303700	-2.64232900	-0.82015900				

5

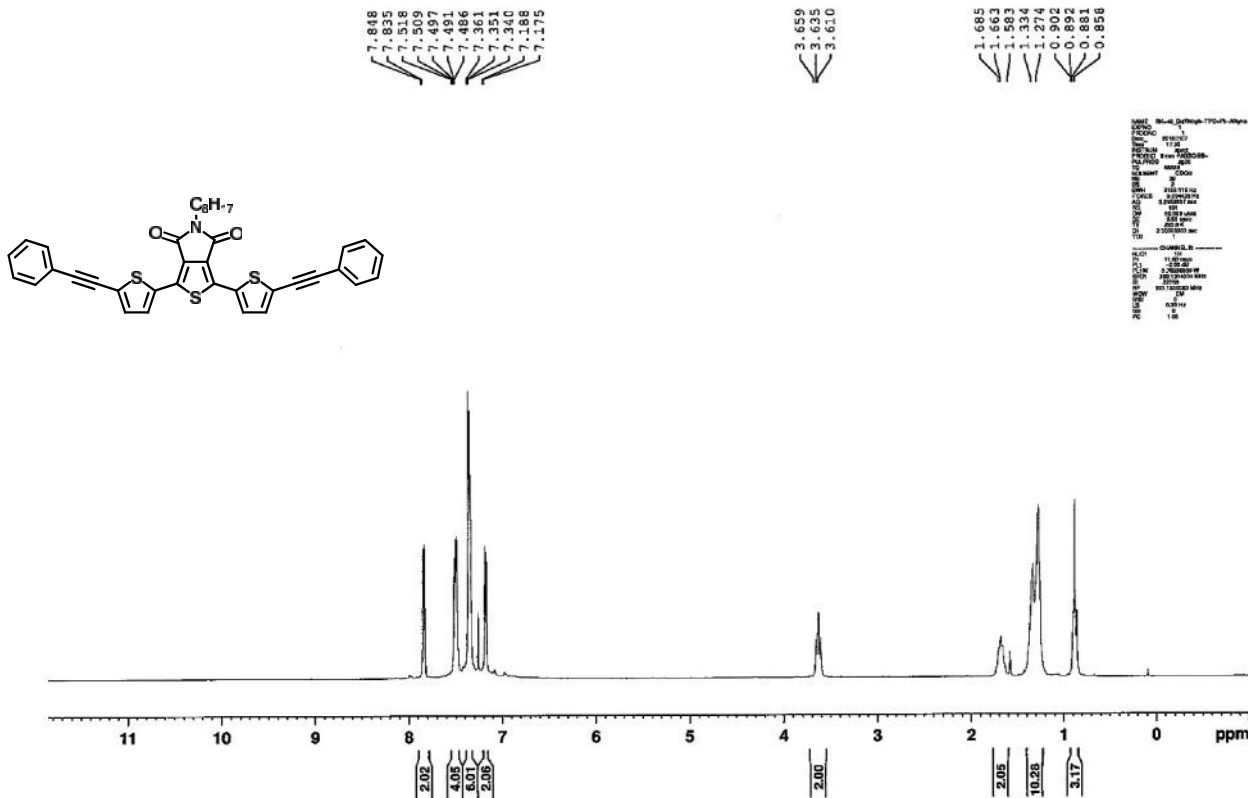


0 1				H	-9.59267700	-2.31765100	0.74496400
C	-1.29467300	-0.55658000	-0.01043600	H	-8.86546400	1.60843600	-0.82949600
C	-0.71328900	0.68795000	-0.00489900	N	10.80718200	-0.06337300	0.04016200
C	0.71071100	0.68875300	0.00448300	N	-10.80713100	-0.06362500	-0.03991500
C	1.29419500	-0.55530800	0.00892200	C	-11.39561600	0.75936800	-1.05269800
C	-1.18489600	2.08374100	-0.00619800	C	-12.36769500	1.71370900	-0.71339400
O	-2.32810800	2.55410900	-0.01119600	C	-11.01788600	0.61833300	-2.39772500
C	1.18084300	2.08388400	0.00712200	C	-12.95187800	2.50424700	-1.70136000
O	2.32516400	2.55325900	0.01270700	H	-12.65945400	1.82528700	0.32282200
N	-0.00360000	2.86062800	0.00078000	C	-11.59393700	1.42487600	-3.37775500
S	0.00056000	-1.77599200	-0.00136000	H	-10.27370100	-0.12103200	-2.66446500
C	2.67007400	-0.96031100	0.01886900	C	-12.56628400	2.36881000	-3.03746600
C	3.14909800	-2.26418900	0.03489700	H	-13.70076000	3.23709700	-1.42385100
S	4.00782600	0.18231900	0.00366600	H	-11.29165000	1.30488300	-4.41173600
C	4.55755500	-2.35027200	0.04258700	H	-13.01695300	2.98961500	-3.80235300
H	2.49873000	-3.12884600	0.05244600	C	-11.64003400	-0.61164400	0.98731700
C	5.18033000	-1.11219400	0.03113700	C	-12.89651900	-1.15088800	0.66895900
H	5.09751300	-3.28521100	0.08531000	C	-11.21815300	-0.60853000	2.32667200
C	-2.67035700	-0.96246600	-0.02065300	C	-13.71311200	-1.67026200	1.67189000
C	-3.14918700	-2.26629800	-0.03776300	H	-13.22381800	-1.15440600	-0.36268100
S	-4.00799900	0.18028300	-0.00445300	C	-12.03304200	-1.14548300	3.32167400
C	-4.55774400	-2.35239100	-0.04549100	H	-10.25325100	-0.18684300	2.57713200
H	-2.49877500	-3.13092300	-0.05596800	C	-13.28565400	-1.67584900	3.00219600
C	-5.18048800	-1.11434700	-0.03295900	H	-14.68080300	-2.08293700	1.41072100
H	-5.09763100	-3.28735100	-0.08885600	H	-11.69374000	-1.13551300	4.35109200
C	0.00118700	4.32344700	0.00149100	H	-13.91997400	-2.08616700	3.77863100
H	-0.49934100	4.70716500	-0.89193200	C	11.39593900	0.75769200	1.05442800
H	-0.51065700	4.70622200	0.88888100	C	12.36802400	1.71253700	0.71664200
H	1.04827500	4.63248000	0.00807800	C	11.01858100	0.61405900	2.39926500
C	6.61685100	-0.83608000	0.03922900	C	12.95259900	2.50111100	1.70595200
C	7.53886200	-1.80160400	-0.41237900	H	12.65950200	1.82601300	-0.31944900
C	7.13252400	0.39471400	0.49150700	C	11.59502900	1.41864400	3.38068400
C	8.90418200	-1.55593200	-0.40178800	H	10.27441100	-0.12576000	2.66479000
H	7.17682800	-2.75169200	-0.78635900	C	12.56737400	2.36311800	3.04190500
C	8.49633600	0.65186800	0.48721300	H	13.70151300	3.23438200	1.42966000
H	6.45363900	1.15824200	0.85486600	H	11.29307700	1.29667300	4.41453000
C	9.41126200	-0.32063500	0.04370400	H	13.01836700	2.98236500	3.80786400
H	9.59183800	-2.31477000	-0.75076200	C	11.64026000	-0.61046200	-0.98747200
H	8.86627800	1.60735400	0.83438000	C	11.21927900	-0.60469100	-2.32709300
C	-6.61699700	-0.83796500	-0.04068600	C	12.89603100	-1.15136600	-0.66916000
C	-7.53943800	-1.80434900	0.40820800	C	12.03434800	-1.14072600	-3.32245200
C	-7.13220600	0.39419900	-0.48977500	H	10.25492800	-0.18171300	-2.57750900
C	-8.90468400	-1.55814600	0.39809300	C	13.71282800	-1.66980300	-1.67240700
H	-7.17783500	-2.75557600	0.77970000	H	13.22261500	-1.15691700	0.36269900
C	-8.49593400	0.65184500	-0.48493300	C	13.28625300	-1.67277100	-3.00300500
H	-6.45304200	1.15854600	-0.85088500	H	11.69575400	-1.12872300	-4.35208000
C	-9.41122400	-0.32147400	-0.04411900	H	14.67996600	-2.08380000	-1.41129200
				H	13.92072800	-2.08237200	-3.77969100

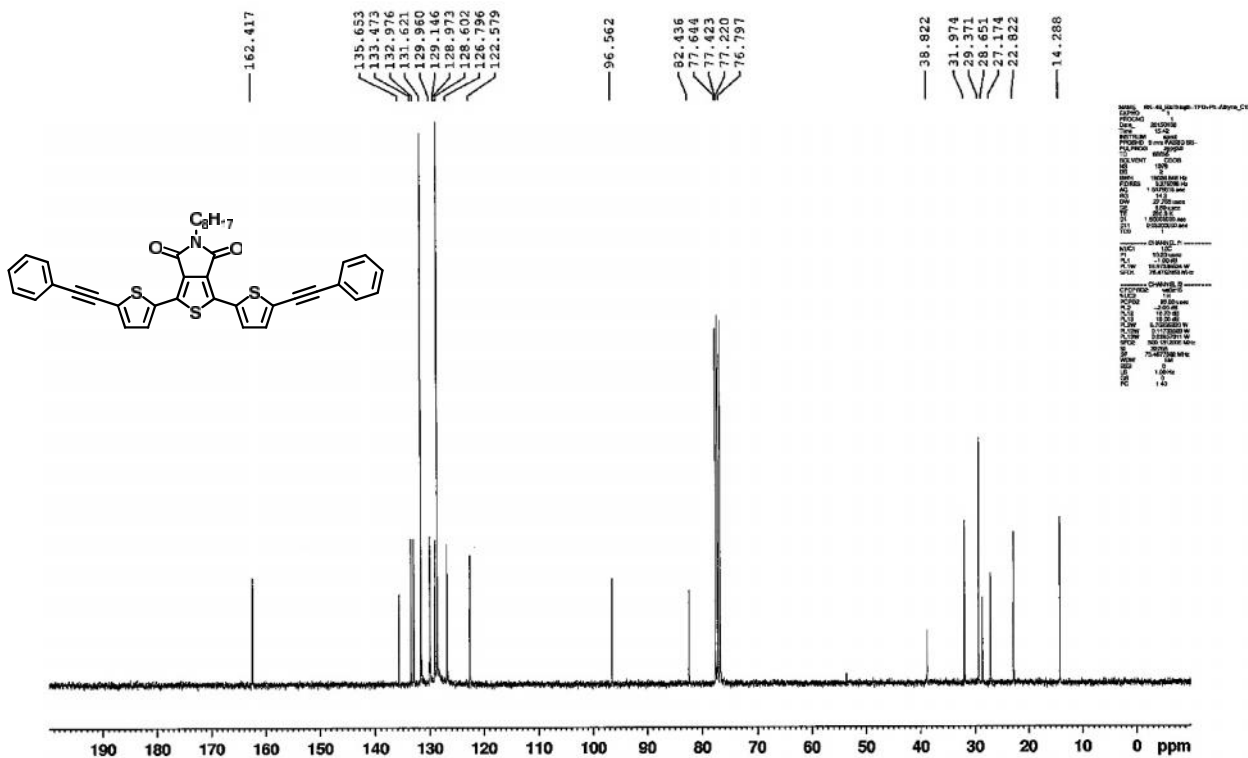
8. ¹H and ¹³C NMR

1,3-bis(5-(phenylethynyl)thiophen-2-yl)- 5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (1)

RK-48_BisThioph-TPD+Ph-Alkyne

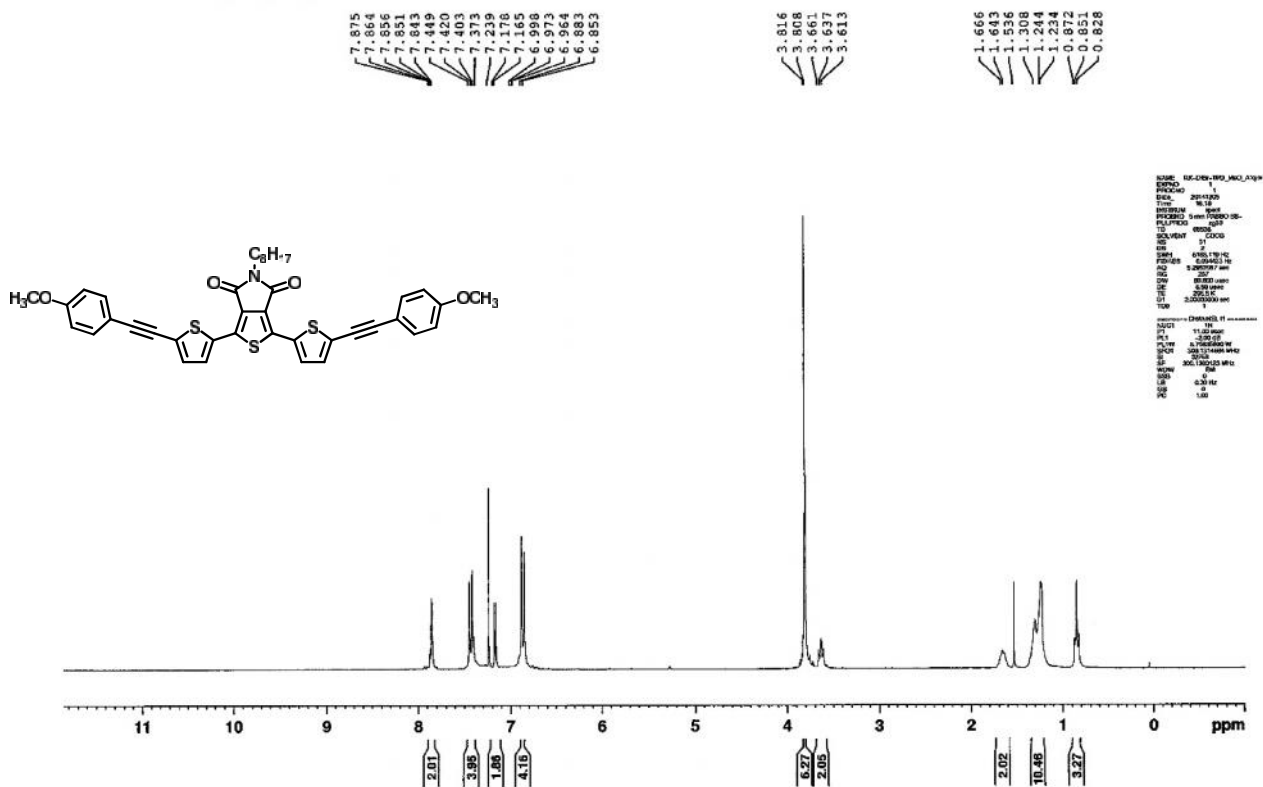


RK-48_BisThioph-TPD+Ph-Alkyne_C13

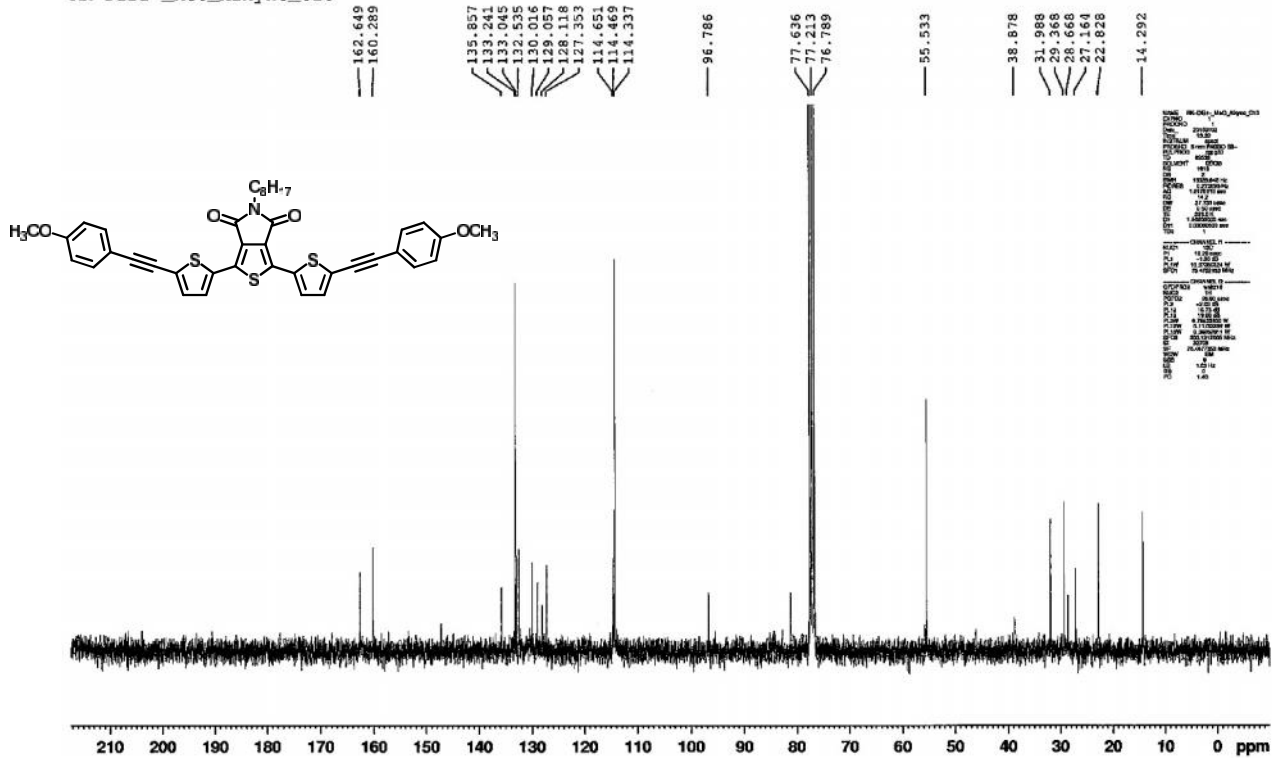


1,3-bis(5-((4-methoxyphenyl)ethynyl)thiophen-2-yl)-5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (2)

RK-DiBr-TPD_MeO_Alkyne

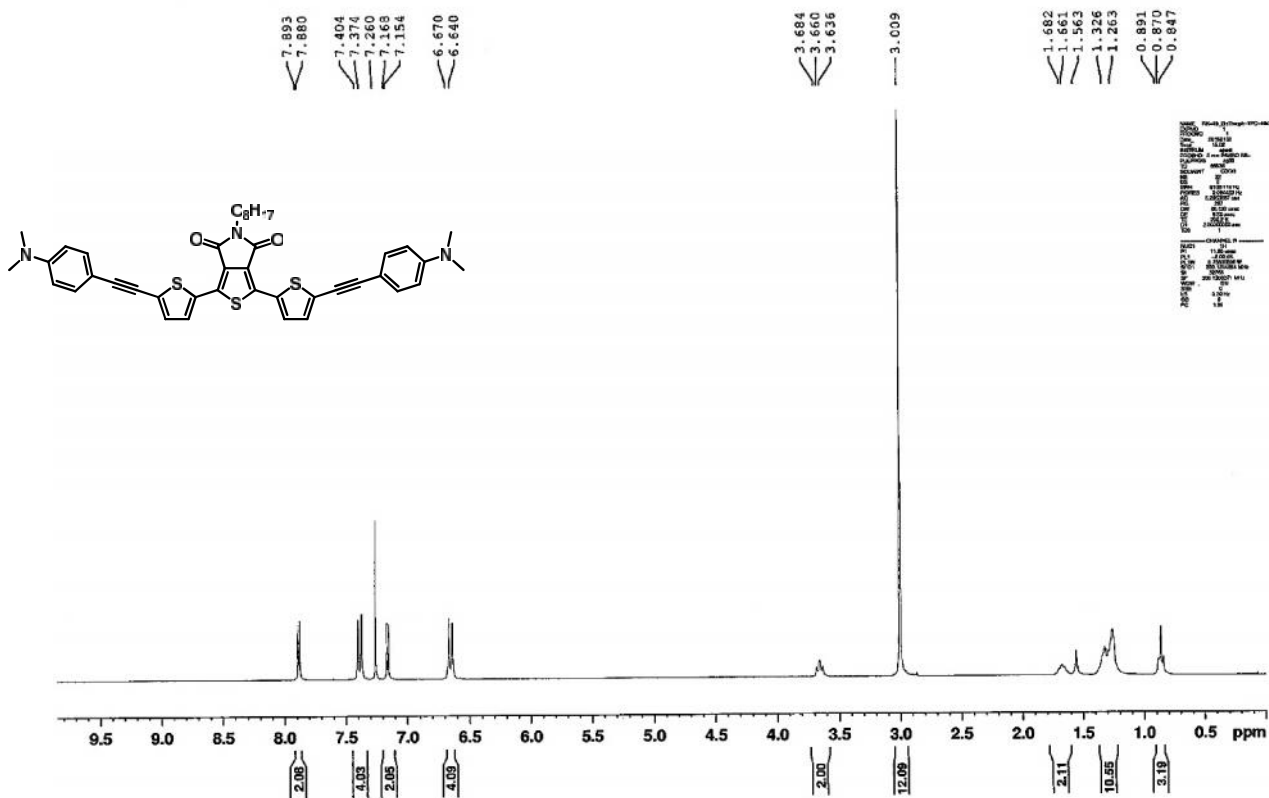


RK-DiBr-MeO_Alkyne_C13

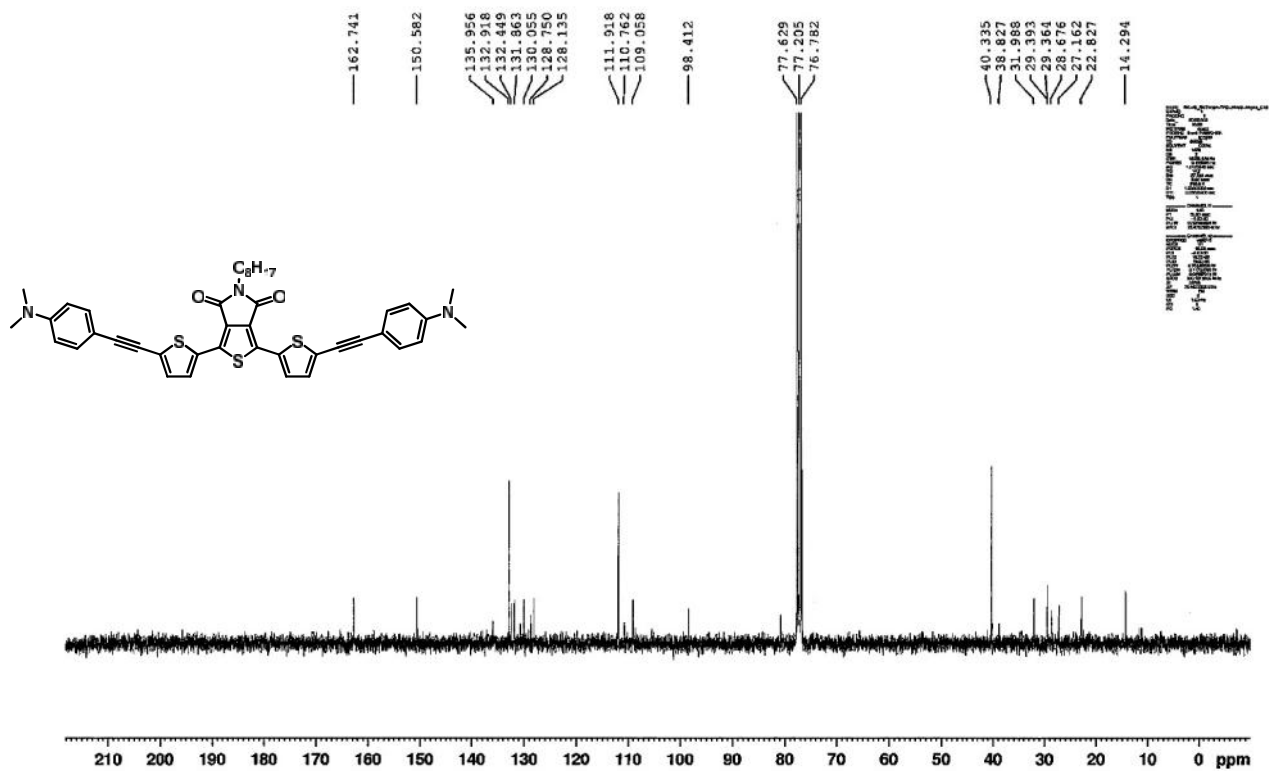


1,3-bis(5-((4-(dimethylamino)phenyl)ethynyl)thiophen-2-yl)-5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (3)

RK-49_BisThioph-TPD+NMe2-Alkyne

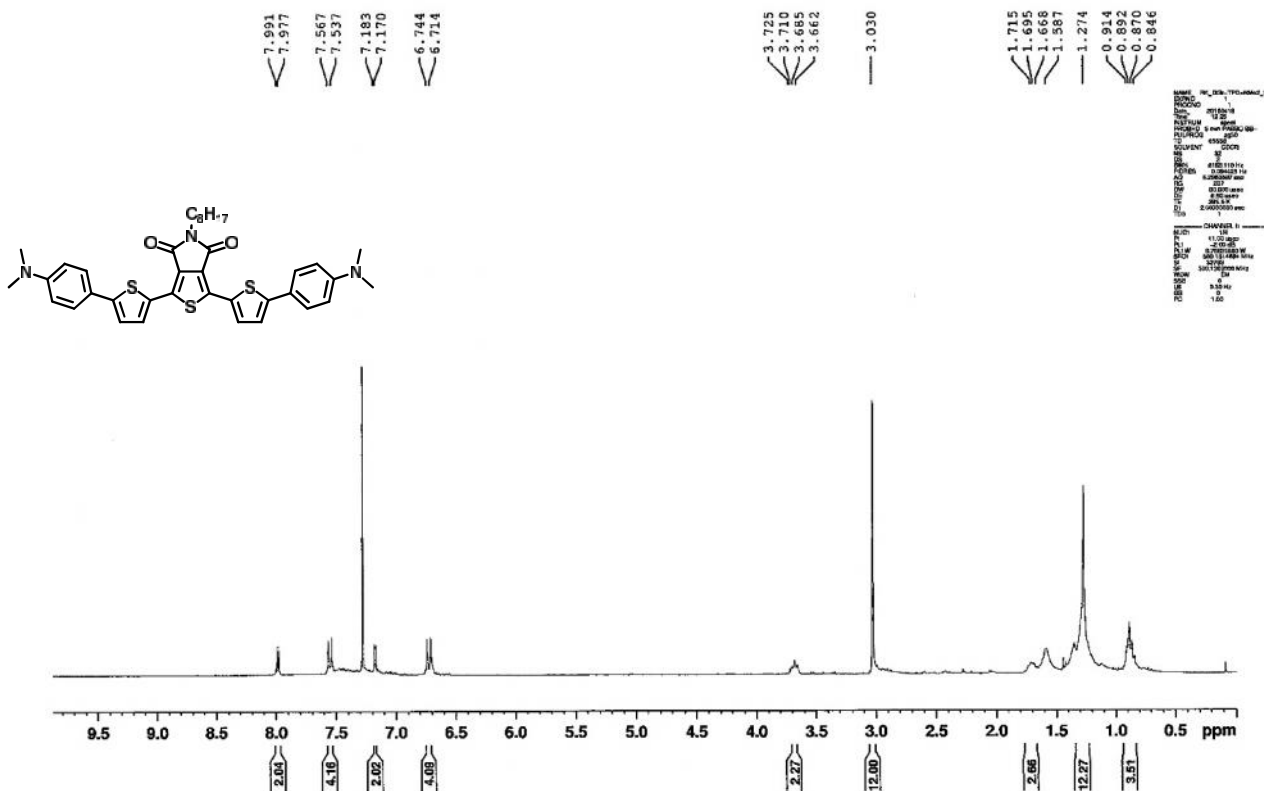


RK-49_BisThioph-TPD+NMe2-Alkyne_C13



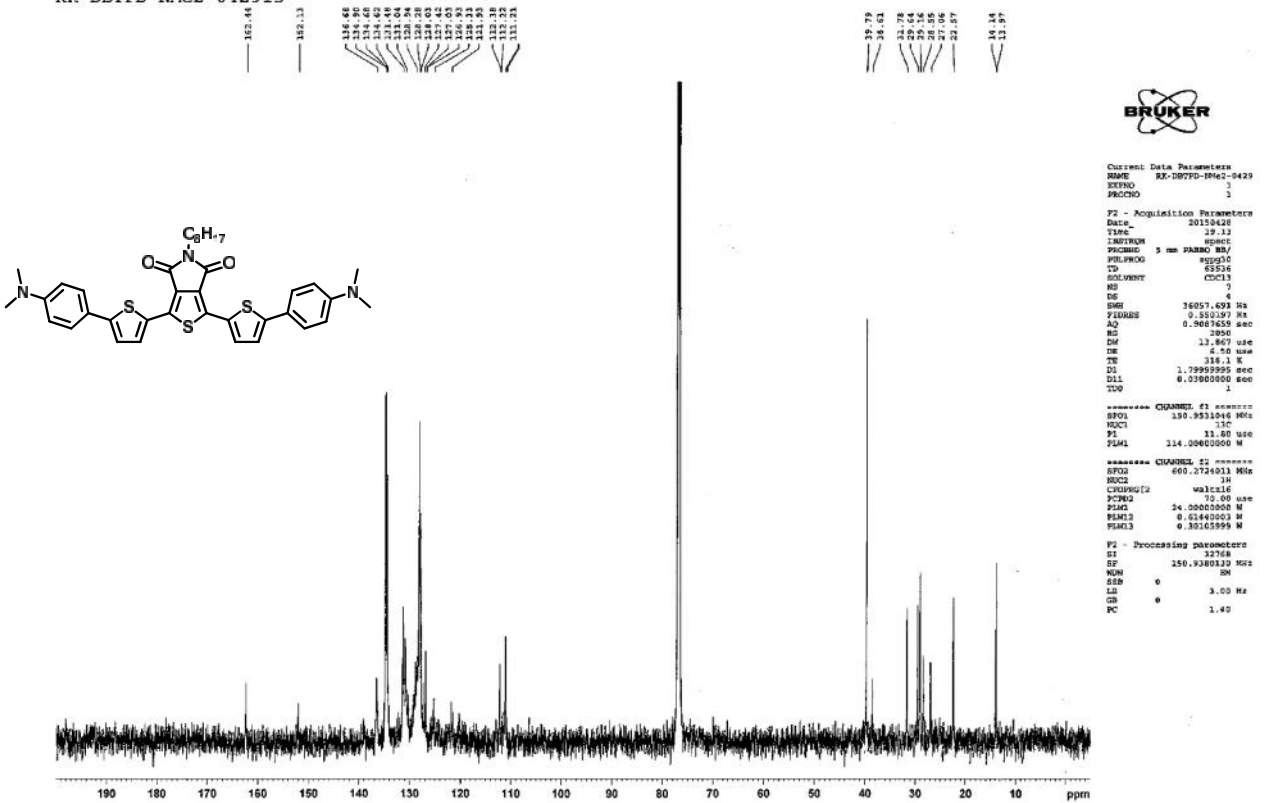
1,3-bis(5-(4-(dimethylamino)phenyl)thiophen-2-yl)-5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (4)

RK_DiBr-TPD+NMe2_Suzuki



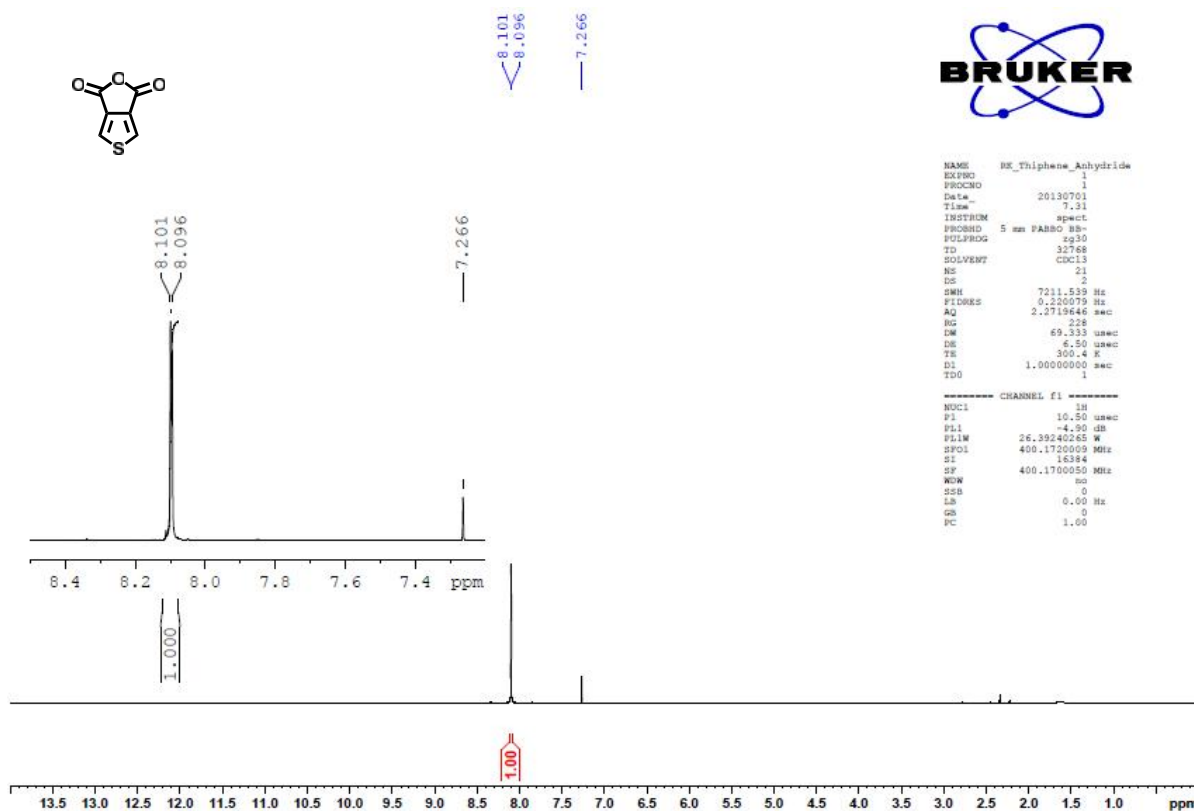
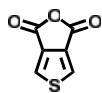
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NAME RK_DiBr-TPD+NMe2_Suzuki
EXPNO 1
PROCNO 1
PROCPS 1
SOLVENT CDCl3
INSTRUM spect
PROBHD 5 mm PABBO MM
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
AQ 1.20000000
RG 256
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.40
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RK-DBTPD-NMe2-042915



```
Current Data Parameters
NAME RK-DBTPD-NMe2-042915
EXPNO 1
PROCNO 1
PROCPS 1
F2 - Acquisition Parameters
Date_ 20150428
TIME 23.12
INSTRUM spect
PROBHD 5 mm PABBO MM
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
RG 256
WDW EM
SSB 0
LB 3.00
GB 0
PC 1.40
===== CHANNEL f1 =====
NUC1 130.9511046 MHz
P1 11.80 use
P1M1 114.0060000 M
===== CHANNEL f2 =====
NUC2 600.2724013 MHz
P2 1.00 use
P2M1 24.0000000 M
P2M2 0.0260000 M
P2M3 0.30105995 M
F2 - Processing parameters
SI 32768
SF 150.930010 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40
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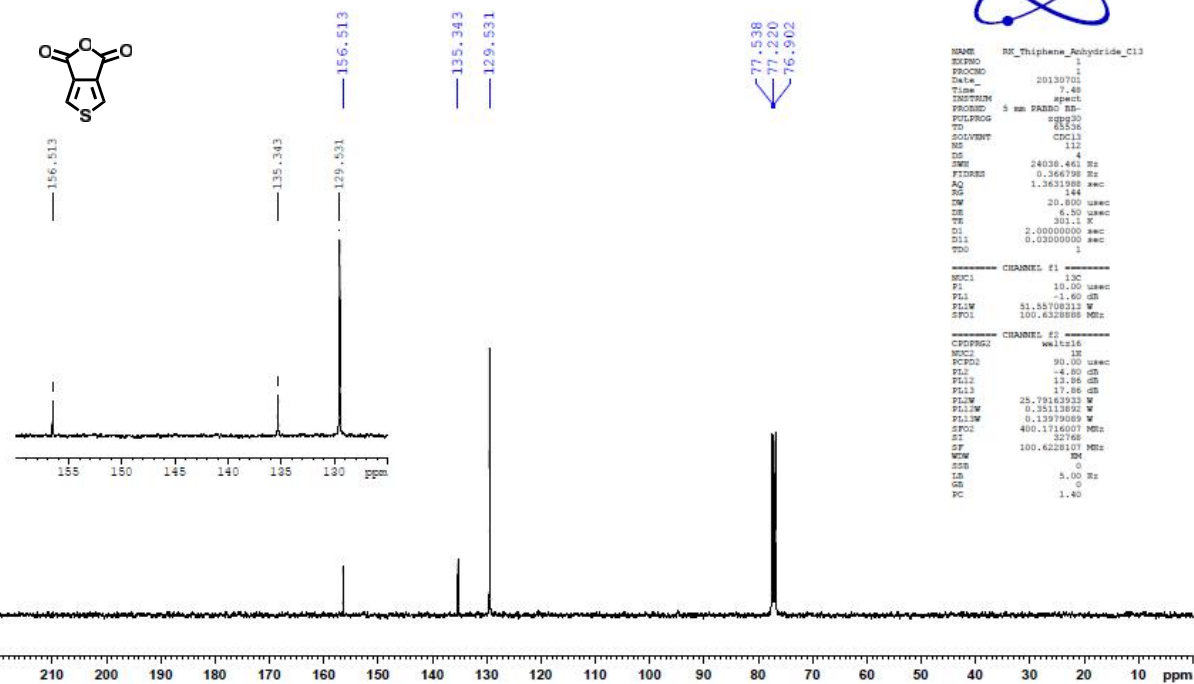

thieno[3,4-c]furan-1,3-dione (7)



```

NAME    BK_Thiophene_Anhydride
EXPNO   1
PROCNO  1
Date_   20130701
Time    7.31
INSTRUM spect
PROBHD  5 mm PABBO BB-
PULPROG zg30
TD       32768
SOLVENT CDCl3
NS       21
DS       2
SWH      7211.539 Hz
FIDRES   0.220079 Hz
AQ       2.2719446 sec
RG       228
DM       69.333 usec
DE       6.50 usec
TE       300.4 K
D1       1.00000000 sec
TD0      1

----- CHANNEL f1 -----
NUC1     1H
P1       10.50 usec
PL1     -4.90 dB
PL1W    26.3924025 W
SFO1    400.1720009 MHz
SI       16384
SF       400.1700050 MHz
WDW      no
SSB      0
LB       0.00 Hz
GB       0
PC       1.00
    
```



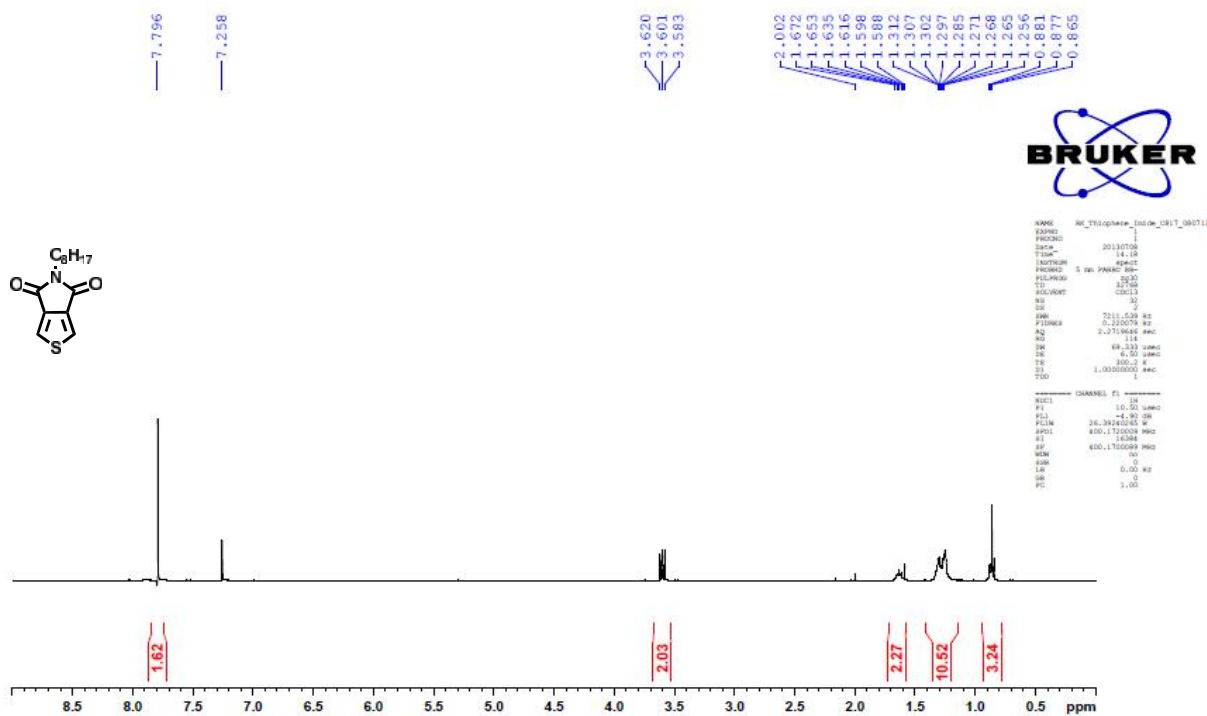
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NAME    BK_Thiophene_Anhydride_C13
EXPNO   1
PROCNO  1
Date_   20130701
Time    7.48
INSTRUM spect
PROBHD  5 mm PABBO BB-
PULPROG zgpg30
TD       65536
SOLVENT CDCl3
NS       112
DS       4
SWH      24038.461 Hz
FIDRES   0.346798 Hz
AQ       1.3631988 sec
RG       144
DM       20.800 usec
DE       6.50 usec
TE       301.1 K
D1       2.00000000 sec
D11     0.03000000 sec
TD0      1

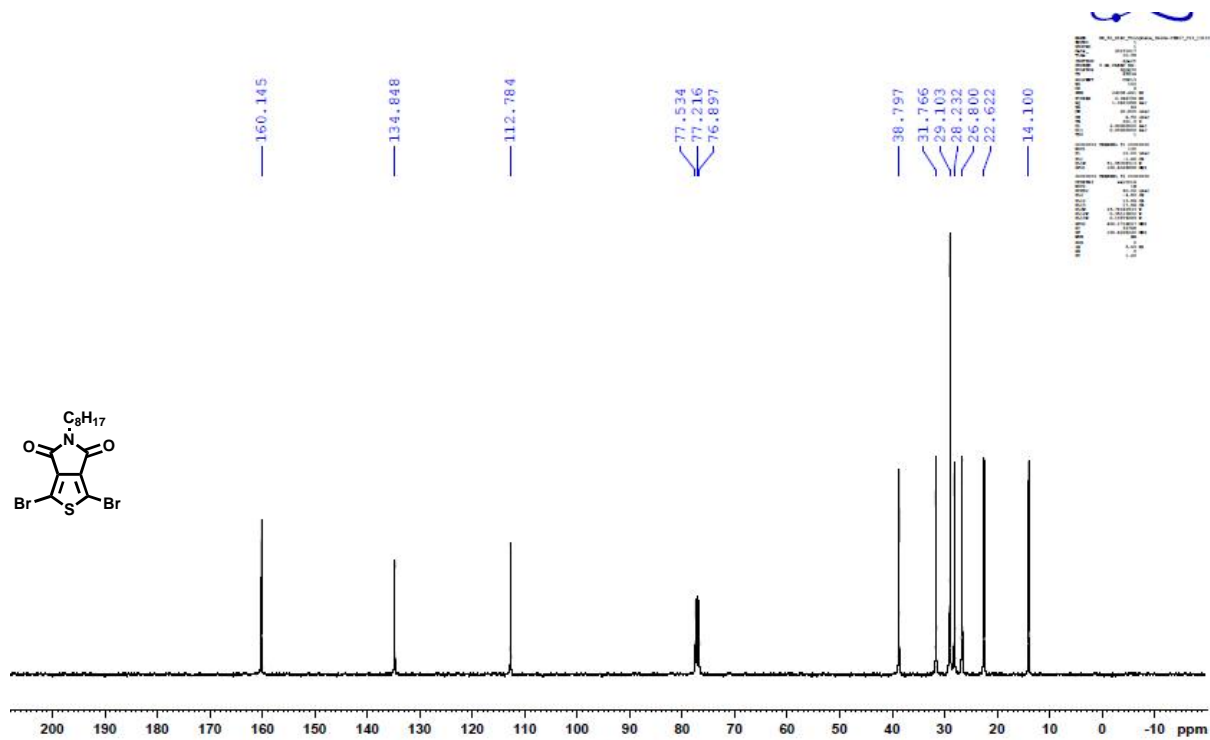
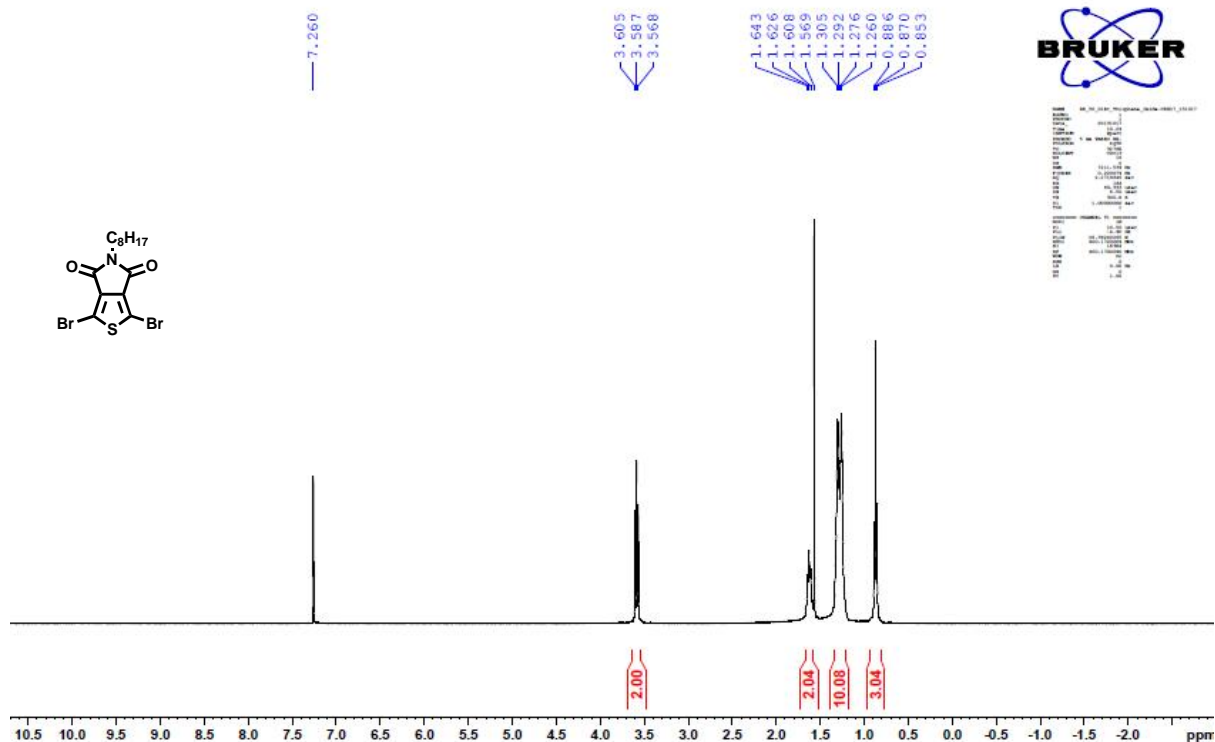
----- CHANNEL f1 -----
MPC1     13C
P1       10.00 usec
PL1     -1.50 dB
PL1W    51.85708213 W
SFO1    100.6228888 MHz

----- CHANNEL f2 -----
CPDPRG2 waltz16
MPC2     1H
PCPD2   90.00 usec
PL2     -4.80 dB
PL12    13.86 dB
PL13    17.86 dB
PL1W    25.79183933 W
PL1W    0.25113852 W
PL1W    0.13979089 W
SFO2    400.1716007 MHz
SI       32768
SF       100.6228101 MHz
WDW      RM
SSB      0
LB       5.00 Hz
GB       0
PC       1.40
    
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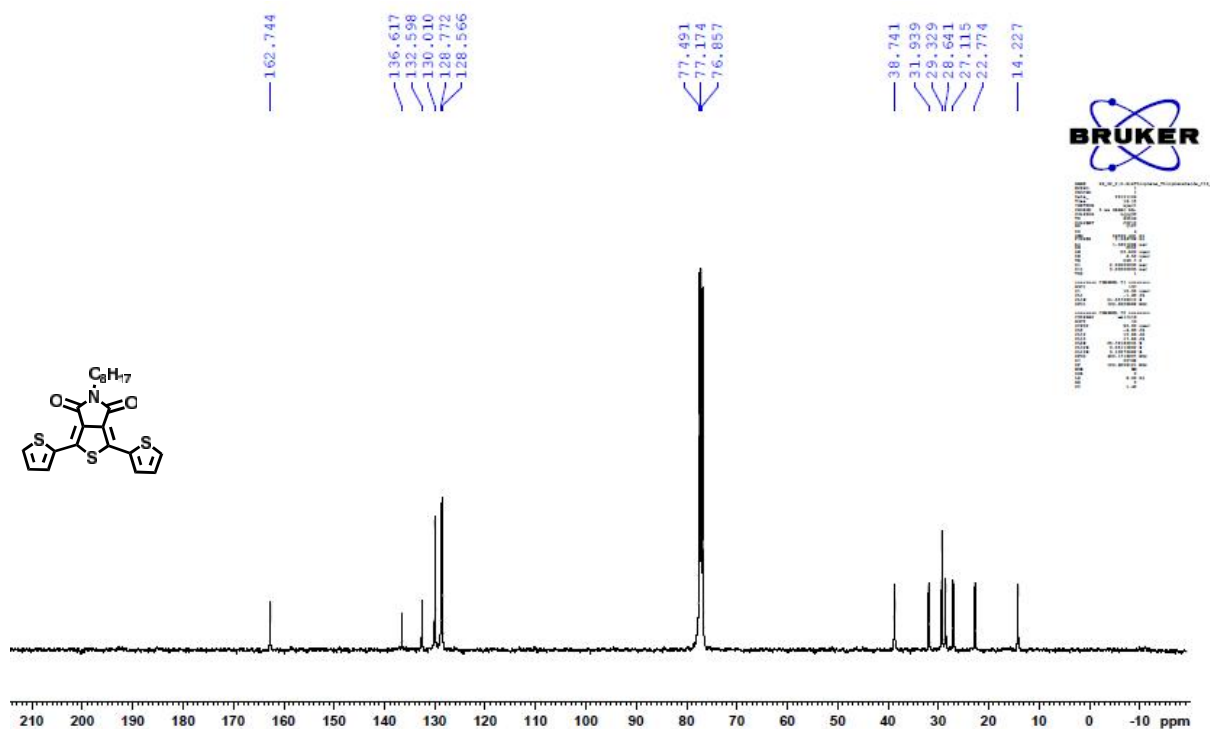
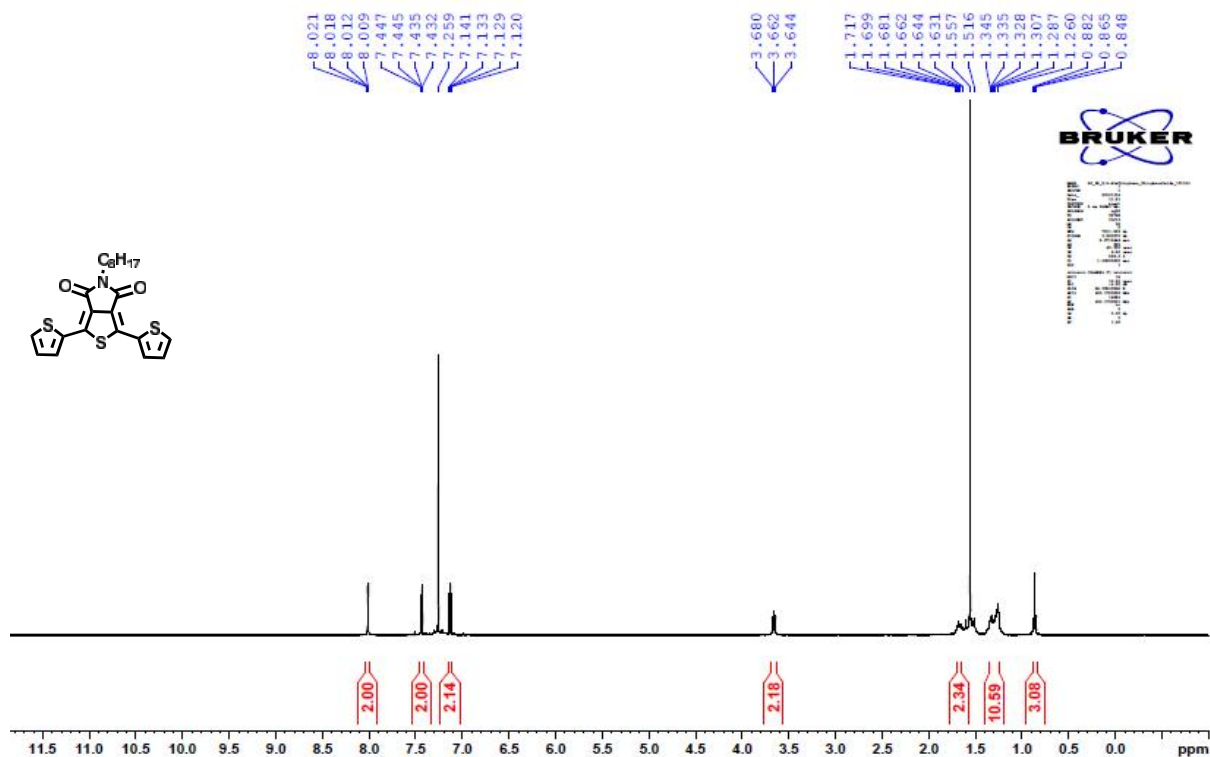
5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (9)



1,3-dibromo-5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (10)



5-octyl-1,3-di(thiophen-2-yl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (11)



1,3-bis(5-bromothiophen-2-yl)-5-octyl-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (12)

