

Supplementary Material

The synthesis and energetic properties of pyridinium and triazolium nitrobenzoyl ylids

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^d*Department of Applied Chemistry, China Agricultural University, Beijing 100193, China*

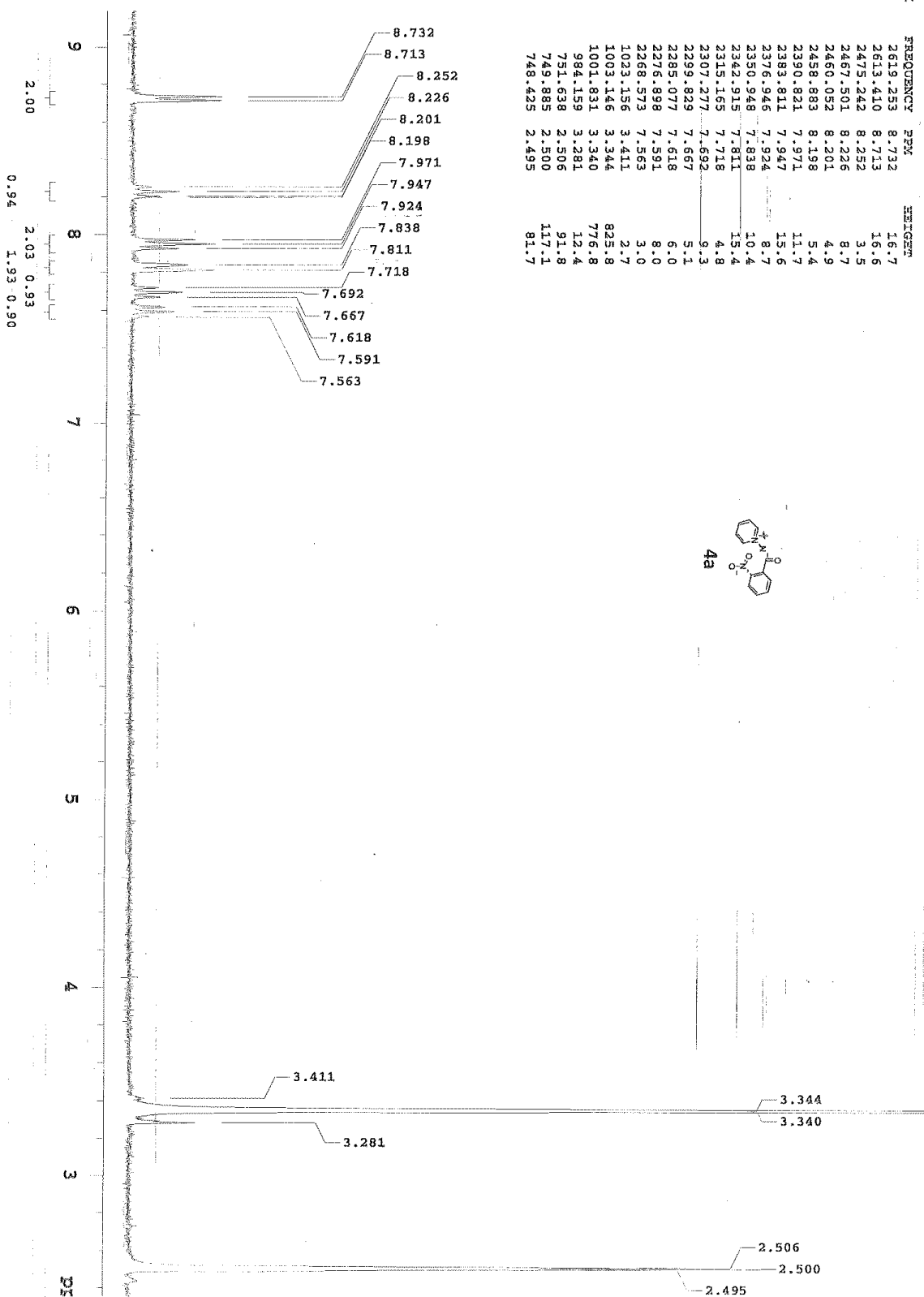
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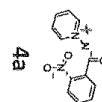
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¹H, ¹³C spectra, elemental analyses for **4a-e**, **6a-e** compounds

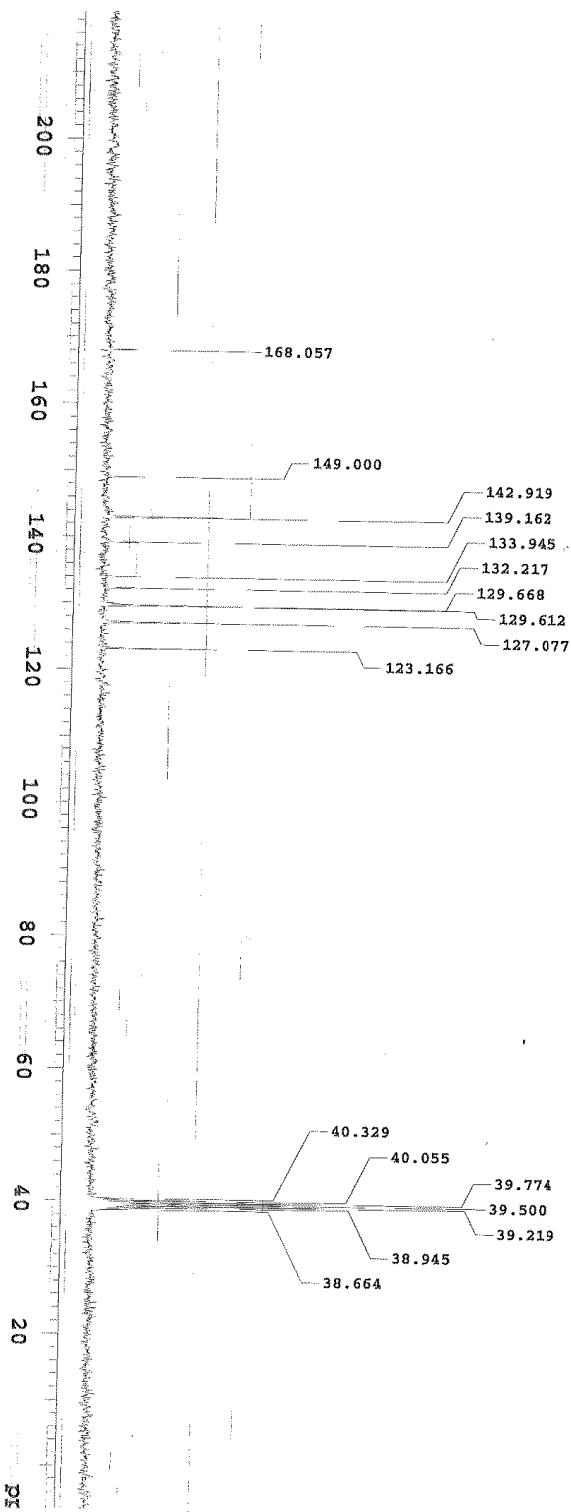
S2



INDEX	FREQUENCY	PPM	INTEGR
1	2619.253	8.732	16.7
2	2613.410	8.713	16.6
3	2475.242	8.252	3.5
4	2467.501	8.226	8.7
5	2460.052	8.201	4.9
6	2458.883	8.198	5.4
7	2390.821	7.971	11.7
8	2383.811	7.947	15.6
9	2376.946	7.924	8.7
10	2350.948	7.838	10.4
11	2342.915	7.811	15.4
12	2315.165	7.718	4.8
13	2307.277	7.692	9.3
14	2299.829	7.667	5.1
15	2285.077	7.618	6.0
16	2276.898	7.591	8.0
17	2268.573	7.563	3.0
18	1023.156	3.411	2.7
19	1001.146	3.344	825.8
20	1001.831	3.340	776.8
21	984.159	3.281	12.4
22	751.638	2.506	91.8
23	749.885	2.500	117.1
24	748.425	2.495	81.7

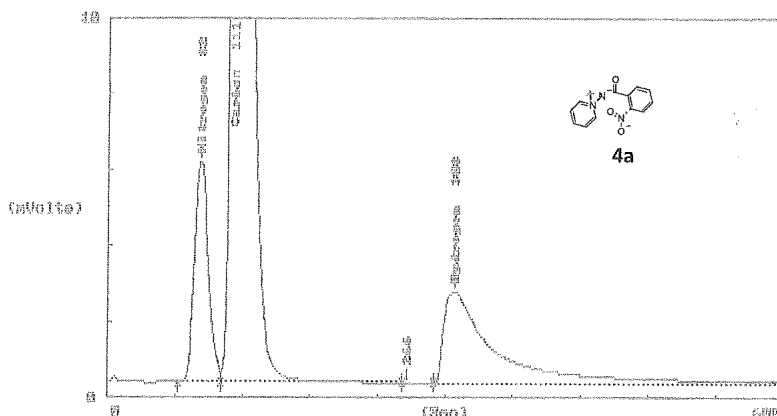


INDEX	FREQUENCY	PMW	HEIGHT
1	12675.454	168.057	4.9
2	11238.074	149.000	6.2
3	10779.426	142.919	33.2
4	10496.081	139.162	15.8
5	10102.576	133.945	6.5
6	9972.290	132.217	18.1
7	9780.039	129.668	22.8
8	9775.802	129.612	19.6
9	9584.611	127.077	37.8
10	9289.614	123.166	18.7
11	3041.725	40.329	7.0
12	3021.070	40.055	18.9
13	2999.885	39.774	37.9
14	2979.230	39.500	44.8
15	2958.046	39.219	38.4
16	2937.391	38.945	19.3
17	2916.206	38.664	6.1



EAGER 200 Stripchart

Sample Ident. : 12 HZ-9 Filename : 288912
 Analysed : 08-11-14 09:37:27 Printed : 08-11-2014 09:47:30



EAGER 200 Peak Integration Report

Instrument name : Instrument #1 Blind drift (fV):-3.4
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-11-14 09:37:27 Printed : 08-11-2014 09:47:30
 Sample Ident. : 12 HZ-9 Filename : 288912
 Sample Weight : 2.173 Calc.method: using 'K. Factors'

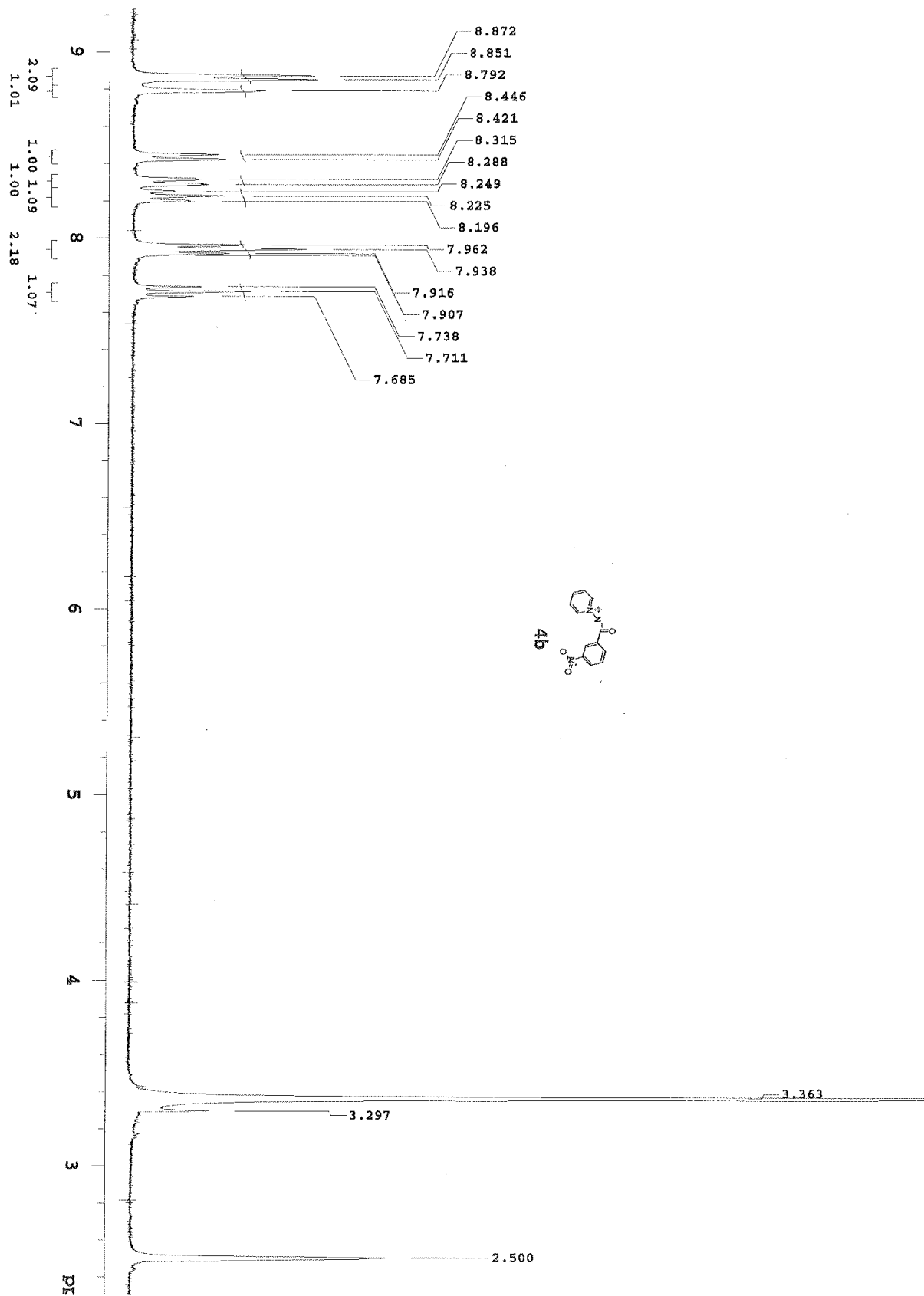
No. (#)	Type (#)	Start (Sec)	End (Sec)	Ret Time (Sec)	Height (fV)	Area (fV*Sec)	Area % (%)	Name	
1	FU	63	101	82	5787.8	76951	8.09	Nitrogen	
2	FU	101	262	111	50116.3	750819	78.98	Carbon	
3	RS	262	290	266	4.0	58	0.01		
4	RS	290	598	308	2356.3	122875	12.92	Hydrogen	
							950702	100.00	

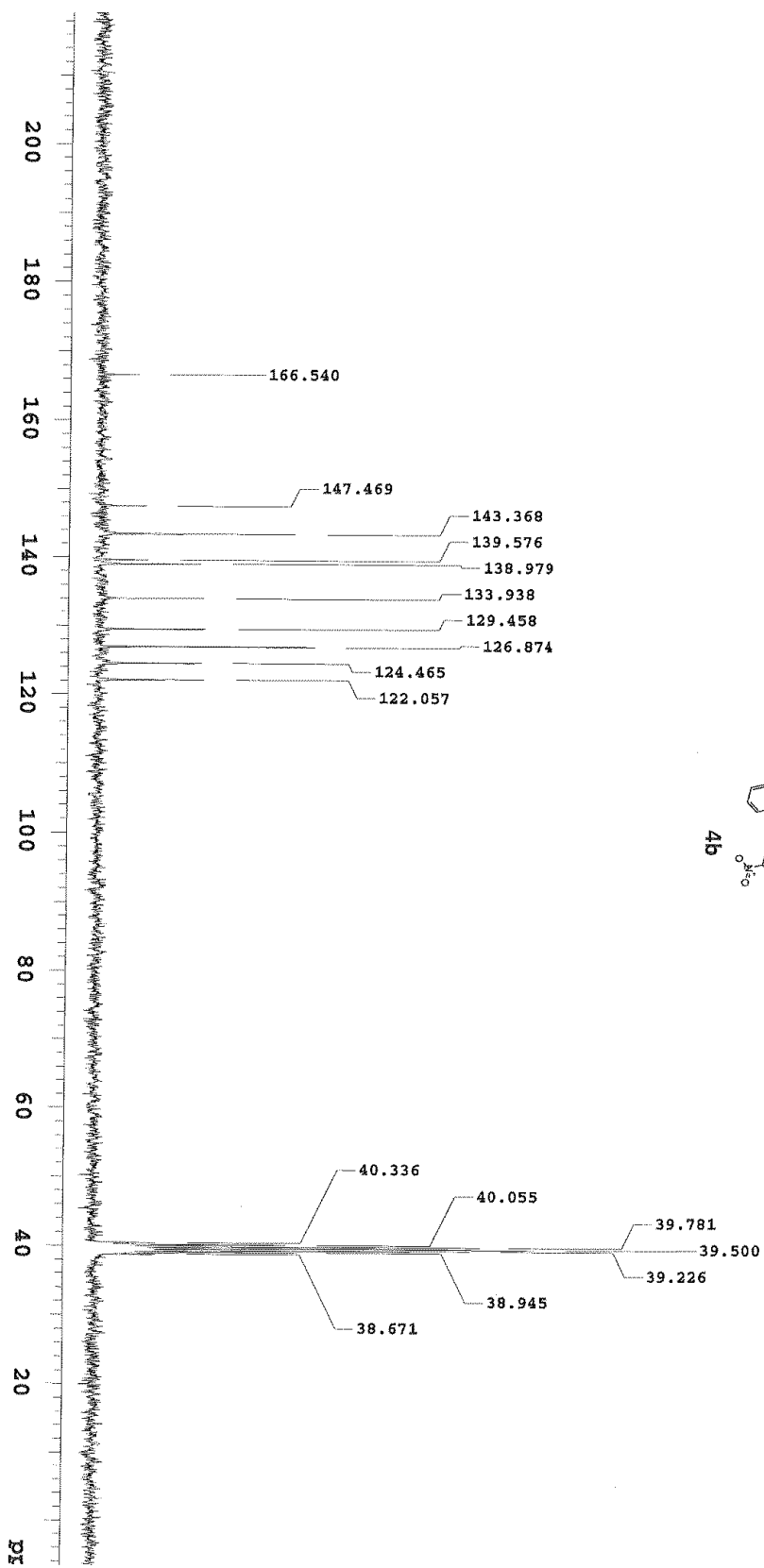
EAGER 200 Unk Report

Instrument name : Instrument #1 Blind drift (fV):-3.4
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-11-14 09:37:27 Printed : 08-11-2014 09:47:30
 Sample Ident. : 12 HZ-9 Filename : 288912
 Sample Weight : 2.173 Calc.method: using 'K. Factors'

Pk. (#)	Ret Time (Sec)	Area (fV*Sec)	Element % (%)	Area Ratio	Name
1	82	76951	17.205	.975716E+01	Nitrogen
2	111	750819	58.944	.100000E+01	Carbon
4	308	122875	3.474	.611045E+01	Hydrogen

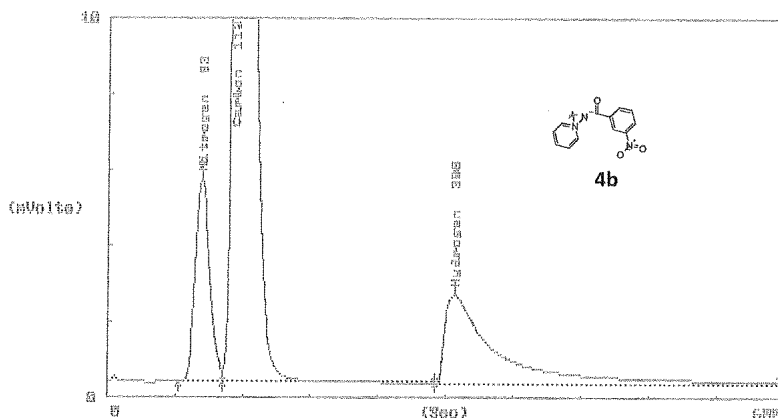
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EAGER 200 Stripchart

Sample Ident. : 15 HZ-20 Filename : 288815
 Analysed : 08-01-14 11:13:24 Printed : 08-01-2014 11:23:25



EAGER 200 Peak Integration Report

Instrument name : Instrument #1 Blind drift (fV): 4.8
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-01-14 11:13:24 Printed : 08-01-2014 11:23:26
 Sample Ident. : 15 HZ-20 Filename : 288815
 Sample Weight : 2.12 Calc.method: using 'K. Factors'

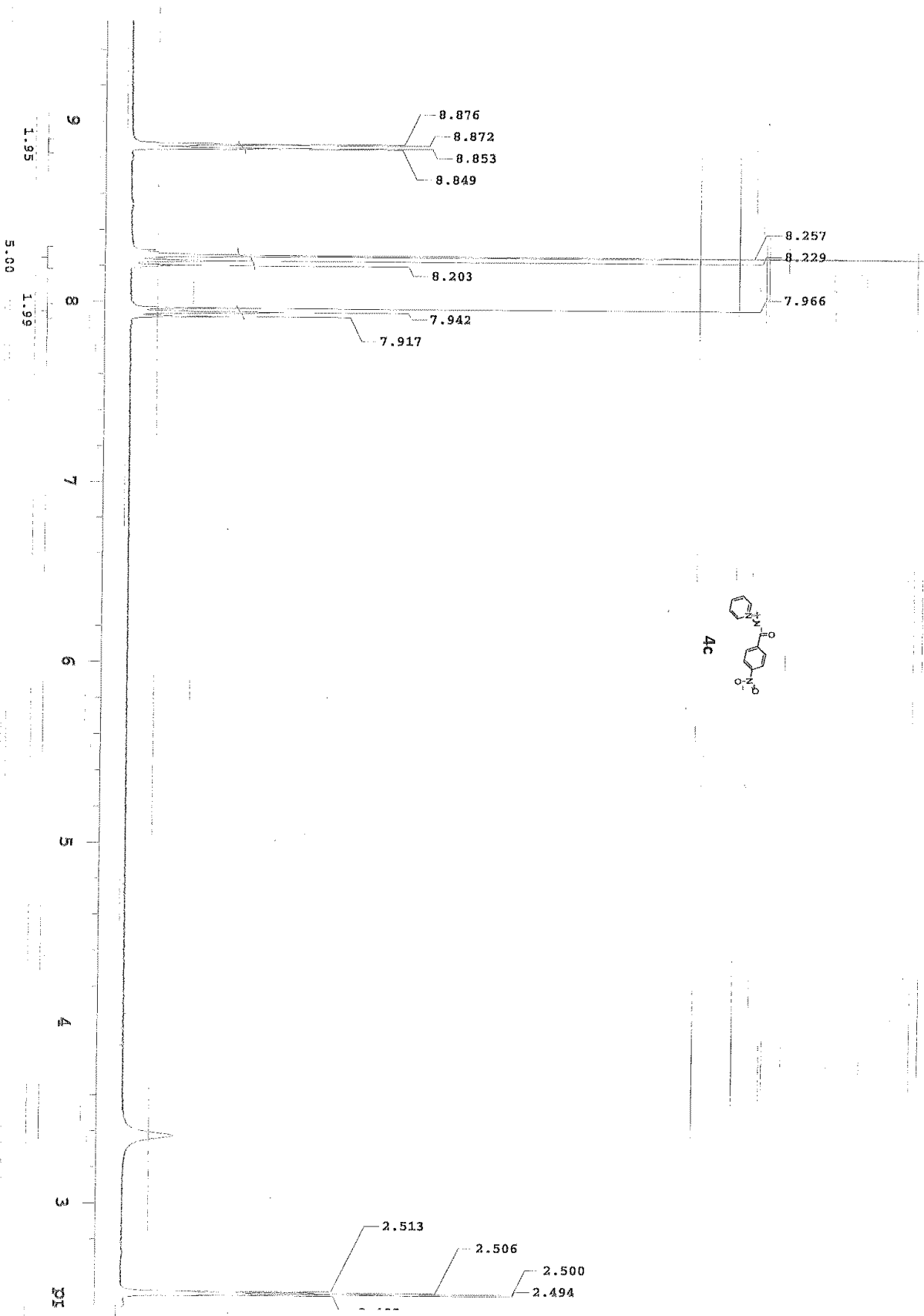
No. (#)	Type	Start (Sec)	End (Sec)	Ret Time (Sec)	Height (fV)	Area (fV*Sec)	Area % (%)	Name
1	FU	63	102	83	5278.2	73898	8.04	Nitrogen
2	FU	102	291	112	47264.7	727924	79.22	Carbon
3	RS	291	597	308	2245.2	117032	12.74	Hydrogen

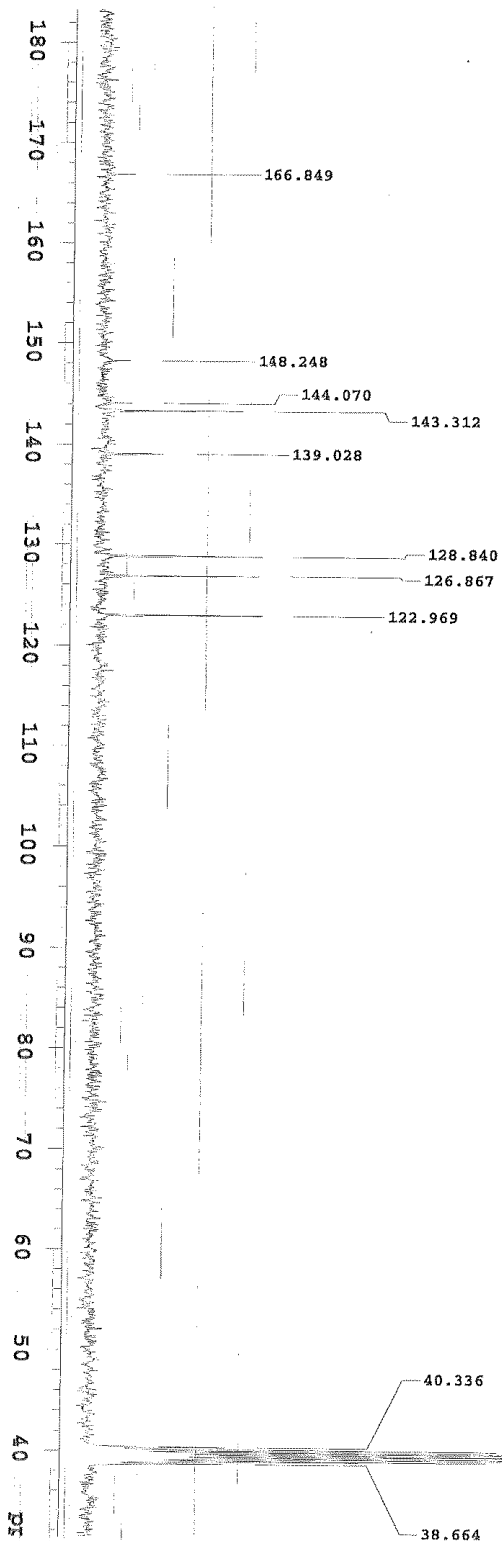
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EAGER 200 Unk Report

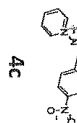
Instrument name : Instrument #1 Blind drift (fV): 4.8
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-01-14 11:13:24 Printed : 08-01-2014 11:23:26
 Sample Ident. : 15 HZ-20 Filename : 288815
 Sample Weight : 2.12 Calc.method: using 'K. Factors'

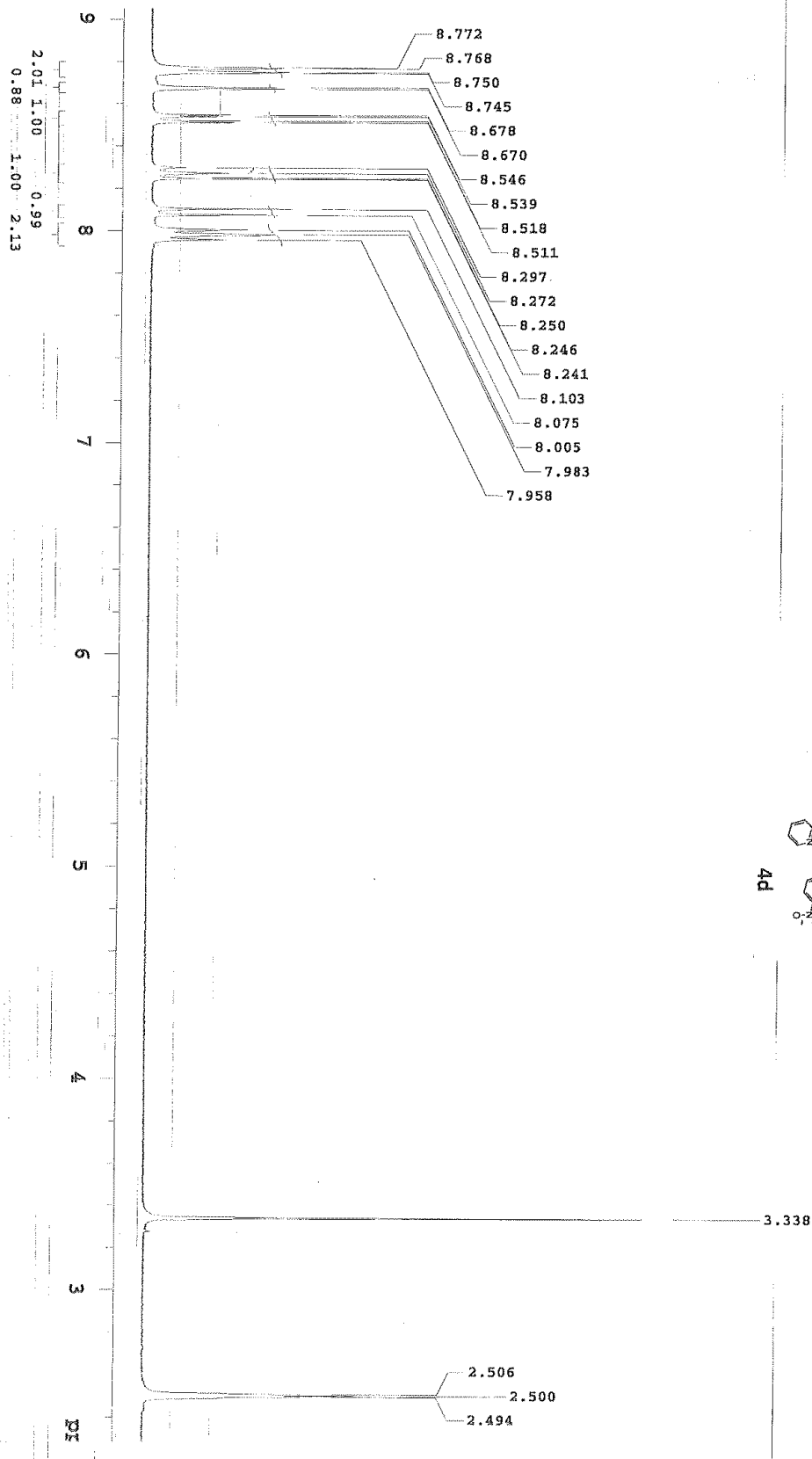
Pk. (#)	Ret Time (Sec)	Area (fV*Sec)	Element % (%)	Area Ratio	Name
1	83	73898	16.603	.985041E+01	Nitrogen
2	112	727924	57.214	.100000E+01	Carbon
3	308	117032	3.284	.621987E+01	Hydrogen

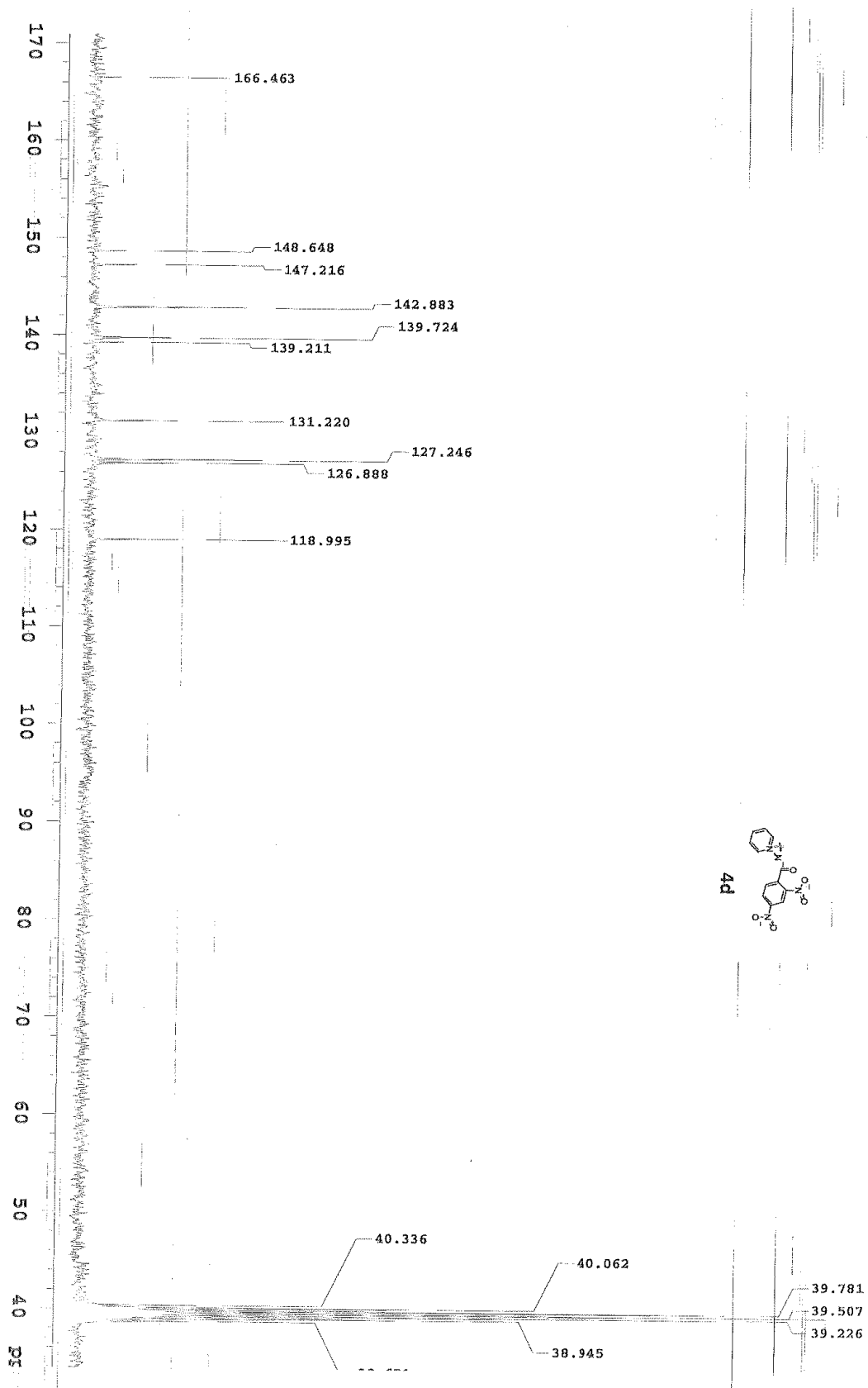




INDEX	FREQUENCY	PPM	HEIGHT
1	12584.360	166.849	4.8
2	11181.406	148.248	4.2
3	10866.284	144.070	4.6
4	10809.085	143.312	22.3
5	10486.019	139.028	9.9
6	9717.545	128.840	25.7
7	9568.722	126.867	25.3
8	9274.785	122.969	25.7
9	3043.255	40.336	21.6
10	3021.070	40.055	65.2
11	2989.885	39.774	127.7
12	2979.230	39.500	148.5
13	2958.046	39.219	126.1
14	2937.391	38.945	63.6
15	2916.206	38.664	21.6

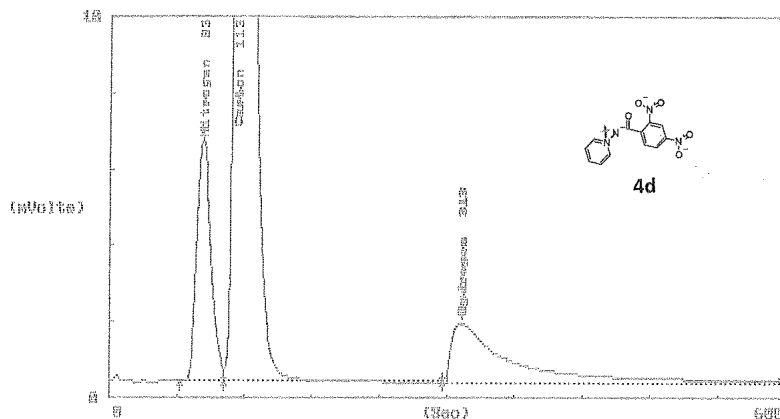






EAGER 200 Stripchart

Sample Ident. : 22 HZ-14 Filename : 289022
 Analysed : 08-18-14 12:18:17 Printed : 08-18-2014 12:28:19



EAGER 200 Peak Integration Report

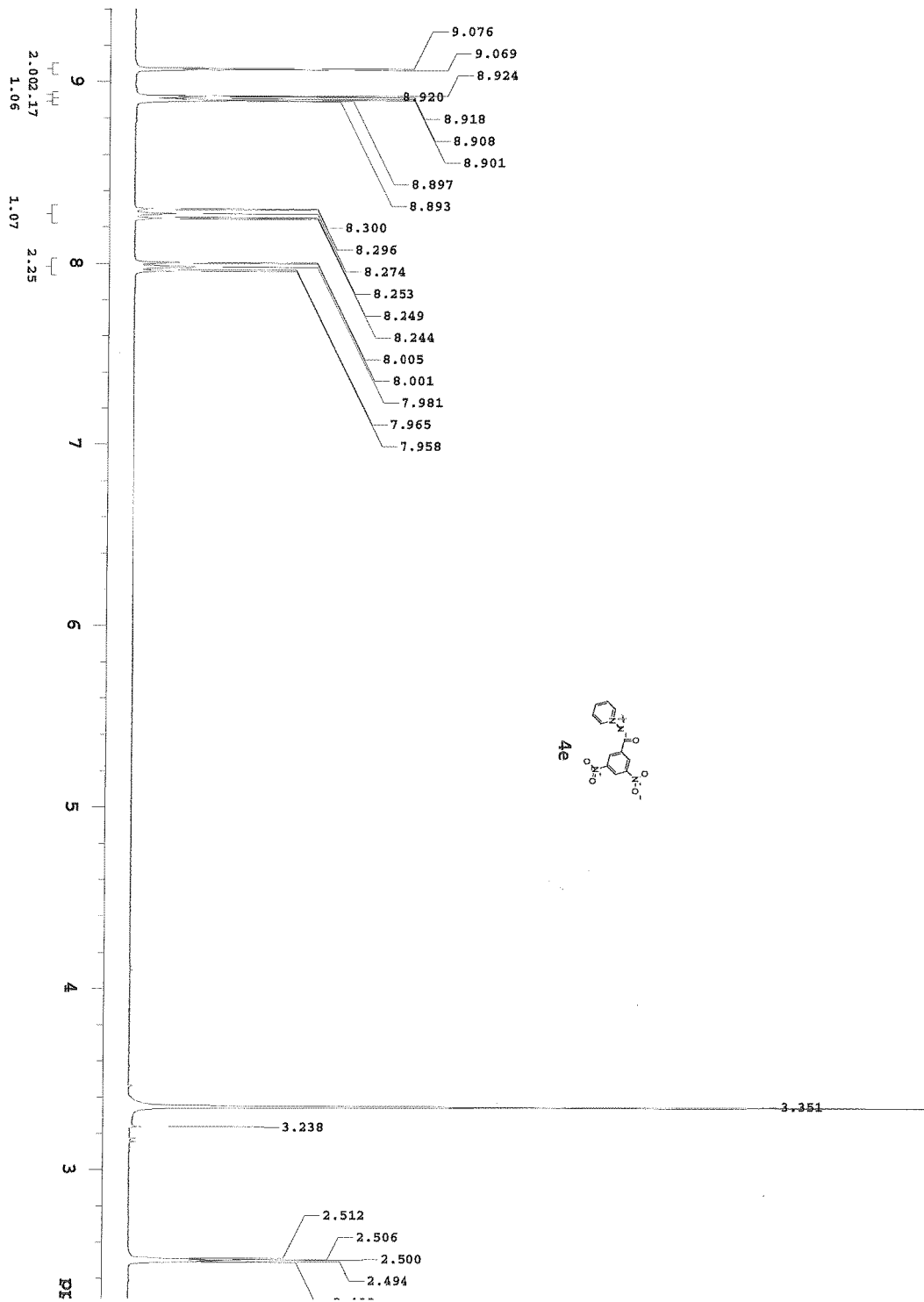
Instrument name : Instrument #1 Blind drift (fV): 2.4
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-18-14 12:18:17 Printed : 08-18-2014 12:28:19
 Sample Ident. : 22 HZ-14 Filename : 289022
 Sample Weight : 2.165 Calc.method: using 'K. Factors'

No. (#)	Type (#)	Start (Sec)	End (Sec)	Ret Time (Sec)	Height (fV)	Area (fV*Sec)	Area % (%)	Name
1	FU	63	102	83	6333.0	86398	10.55	Nitrogen
2	FU	102	296	113	42803.9	644115	78.64	Carbon
3	RS	296	597	313	1518.4	88538	10.81	Hydrogen
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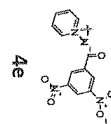
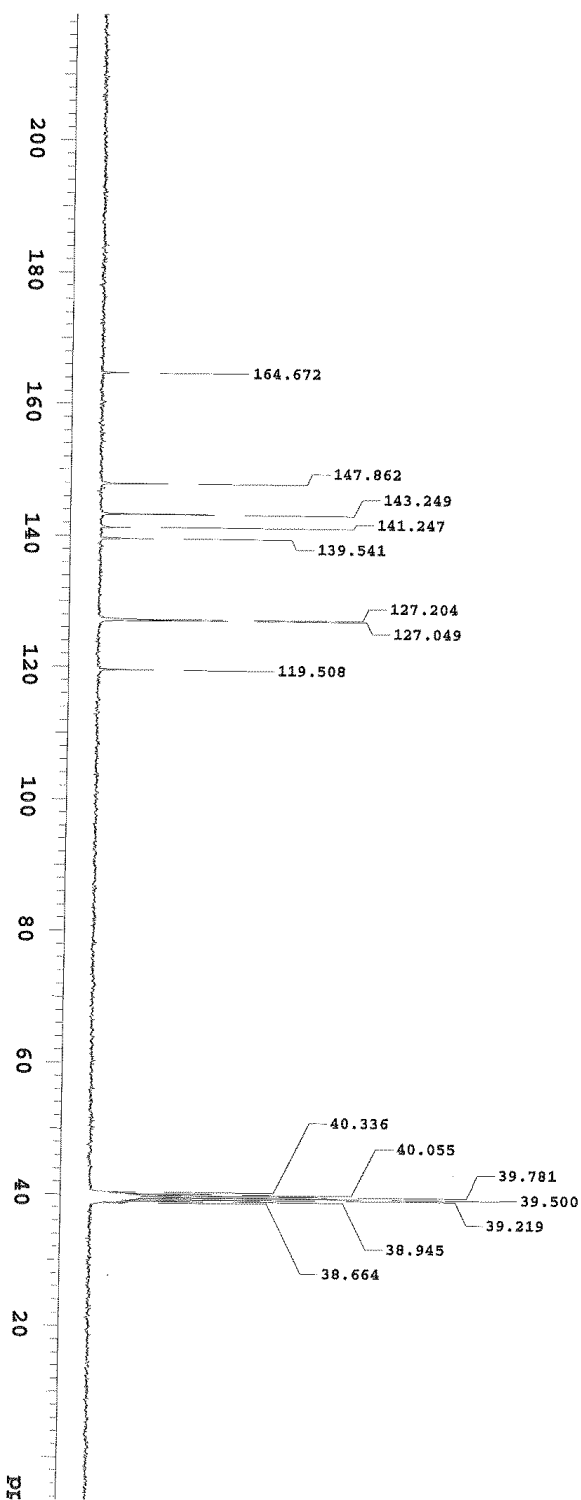
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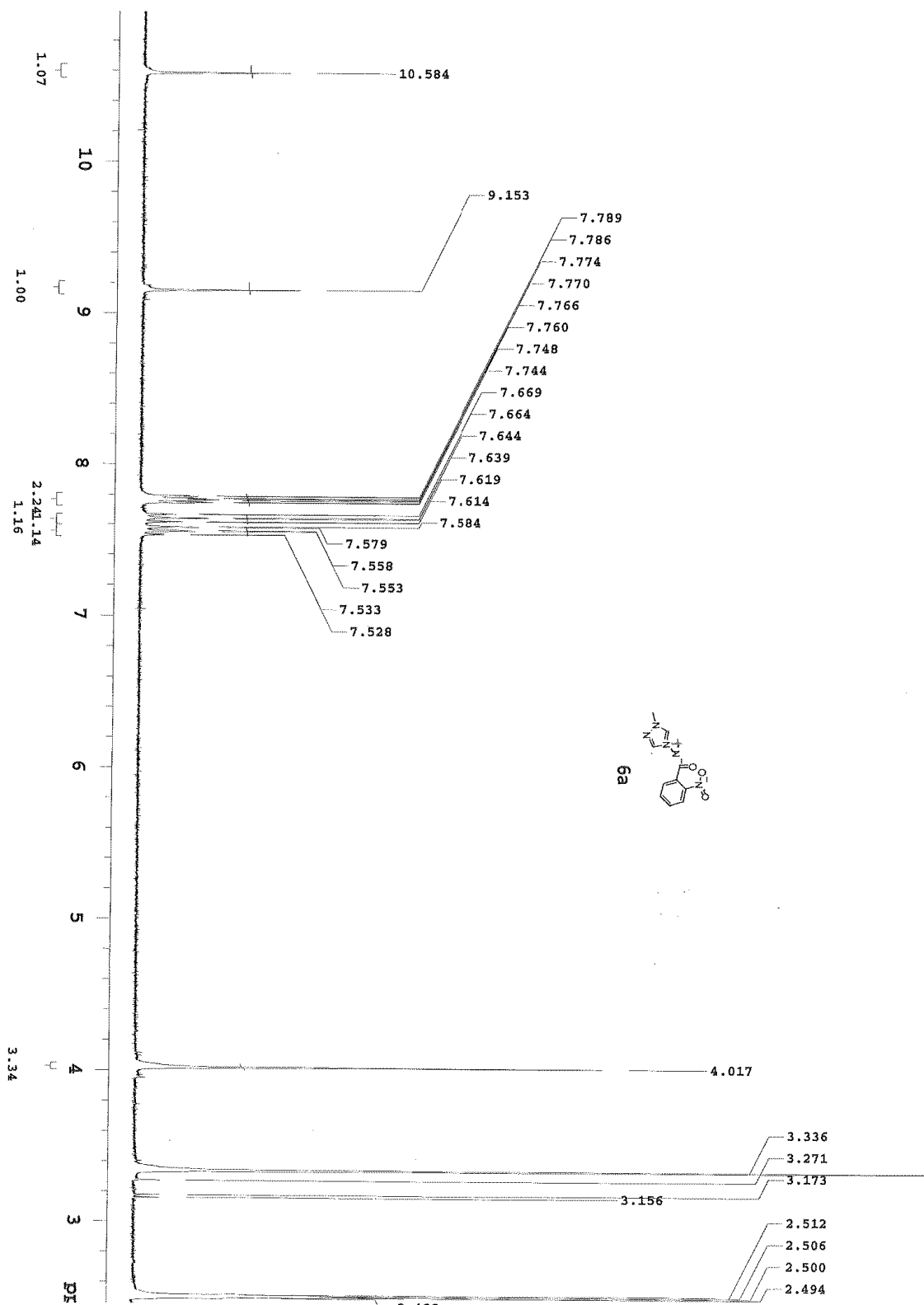
Instrument name : Instrument #1 Blind drift (fV): 2.4
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-18-14 12:18:17 Printed : 08-18-2014 12:28:19
 Sample Ident. : 22 HZ-14 Filename : 289022
 Sample Weight : 2.165 Calc.method: using 'K. Factors'

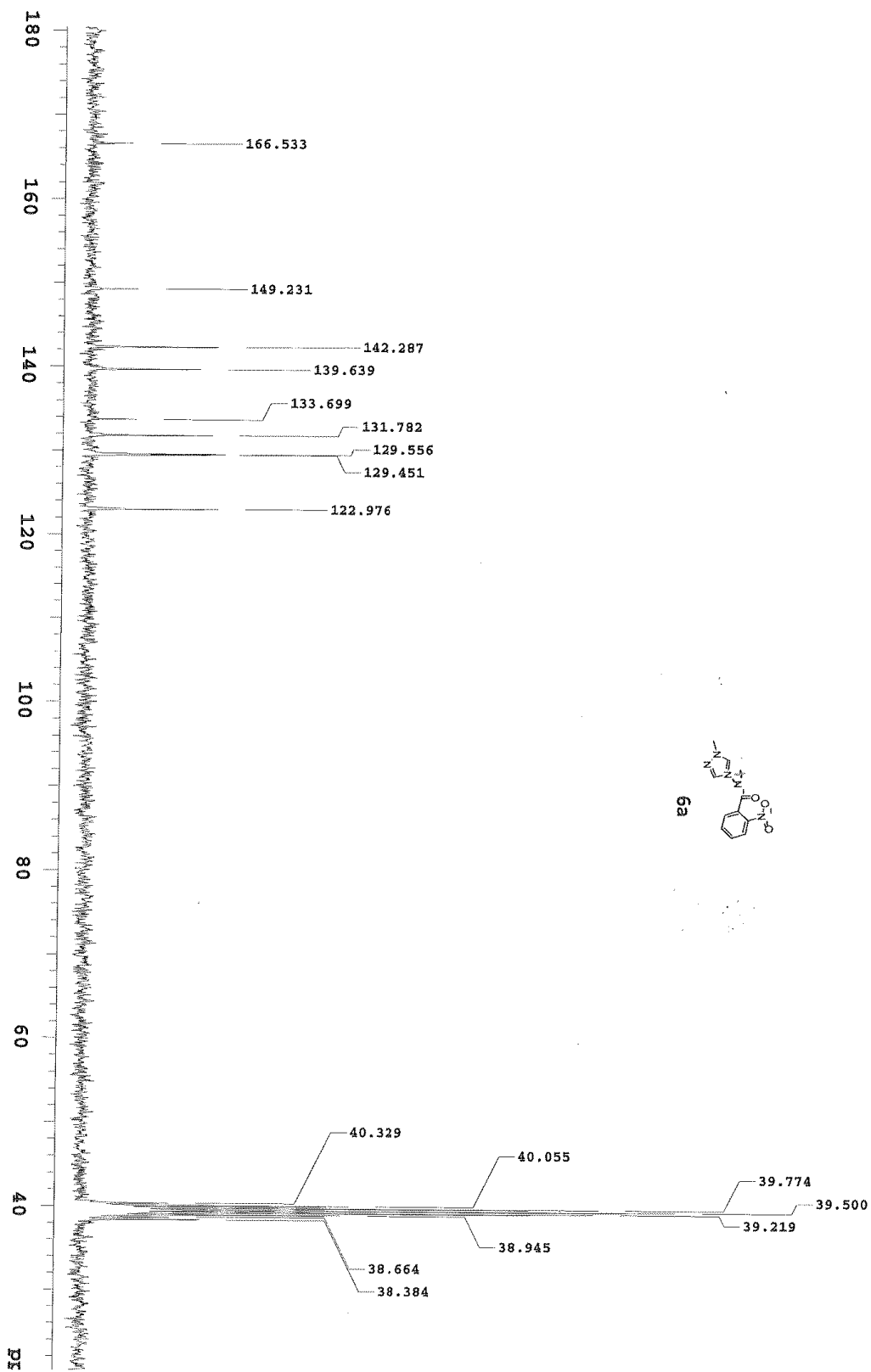
Pk. (#)	Ret Time (Sec)	Area (fV*Sec)	Element % (%)	Area Ratio	Name
1	83	86398	19.125	.745521E+01	Nitrogen
2	113	644115	50.056	.100000E+01	Carbon
3	313	88538	2.483	.727505E+01	Hydrogen



INDEX	FREQUENCY	PPM	HEIGHT
1	12420.179	164.672	4.4
2	1152.277	147.862	11.1
3	10804.318	143.249	18.9
4	10653.378	141.247	4.9
5	10524.681	139.541	8.7
6	9594.144	127.204	20.6
7	9582.492	127.049	21.3
8	9013.684	119.508	9.2
9	3042.255	40.336	7.3
10	3021.070	40.055	20.1
11	3000.415	39.781	39.1
12	2979.230	39.500	44.8
13	2958.046	39.219	37.3
14	2937.391	38.945	18.7
15	2916.206	38.664	6.2

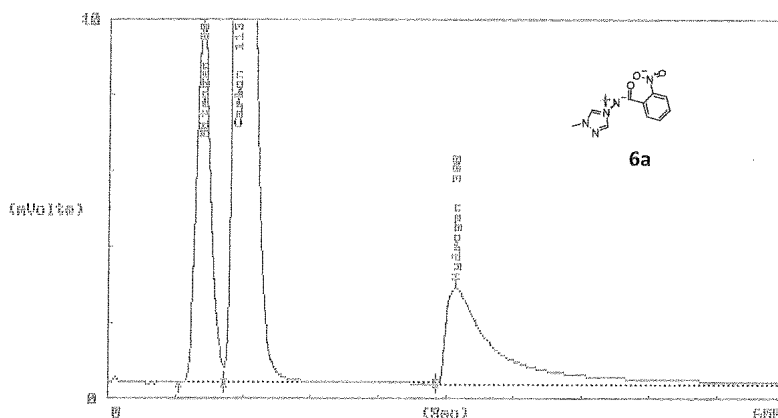






EAGER 200 Stripchart

Sample Ident. : 16 HZ-21 Filename : 288816
 Analysed : 08-01-14 11:23:26 Printed : 08-01-2014 11:33:29



EAGER 200 Peak Integration Report

Instrument name : Instrument #1 Blind drift (fV): 4
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-01-14 11:23:26 Printed : 08-01-2014 11:33:29
 Sample Ident. : 16 HZ-21 Filename : 288816
 Sample Weight : 2.171 Calc.method: using 'K. Factors'

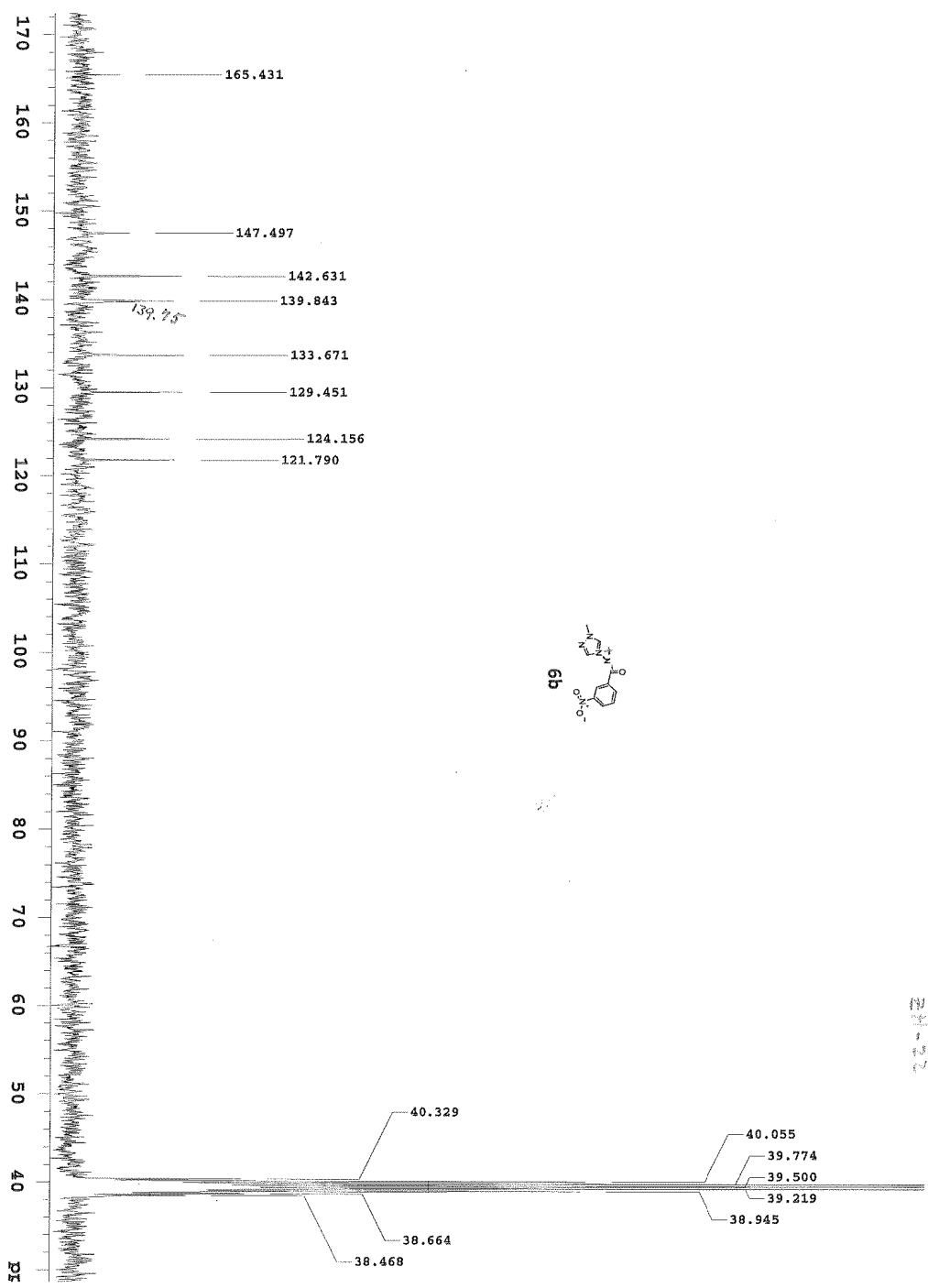
No. (#)	Type (#)	Start (Sec)	End (Sec)	Ret Time (Sec)	Height (fV)	Area (fV*Sec)	Area % (%)	Name
1	FU	63	103	83	9426.7	130375	14.69	Nitrogen
2	FU	103	291	113	41837.4	632321	71.25	Carbon
3	RS	291	598	308	2447.2	124802	14.06	Hydrogen

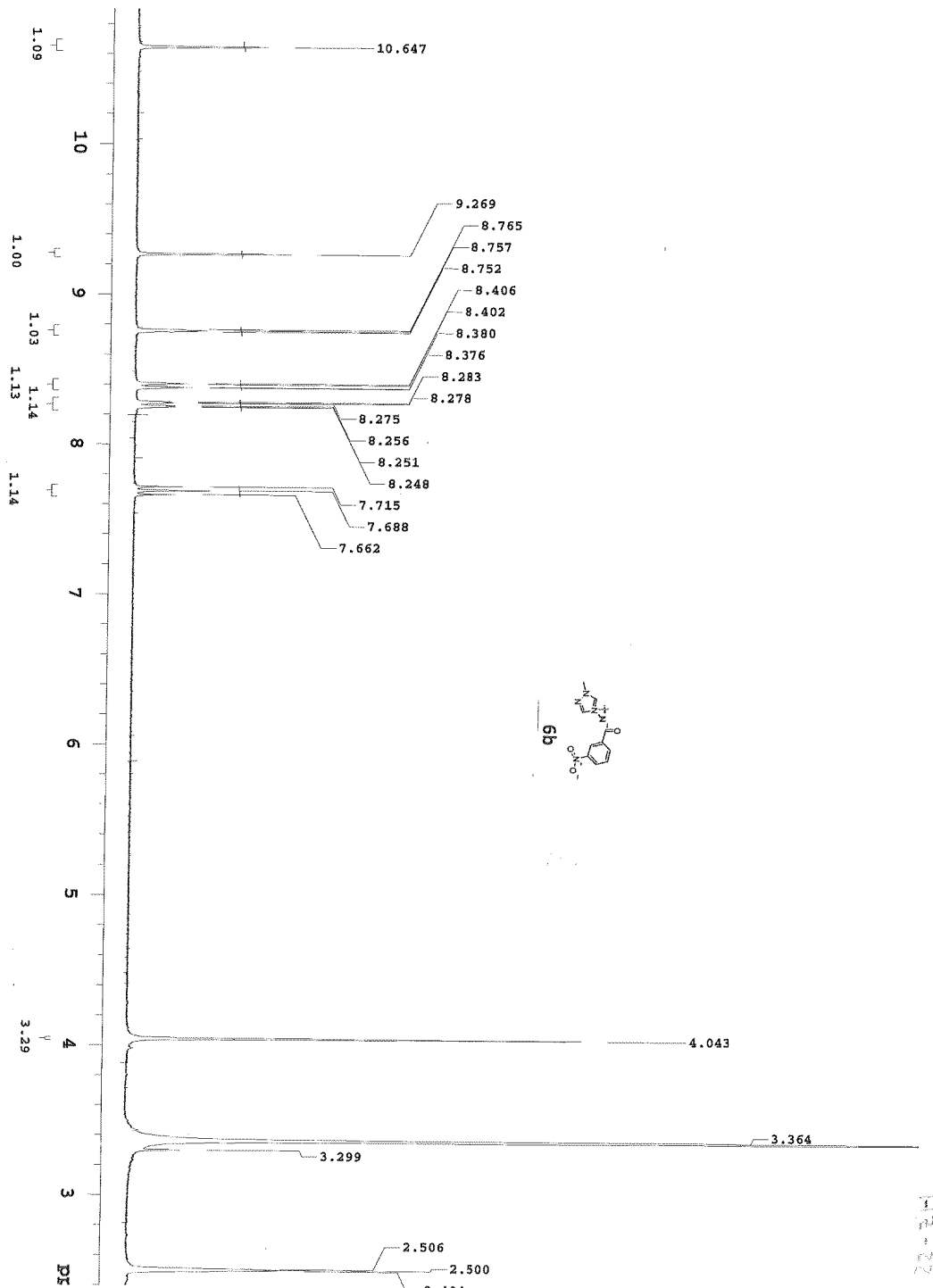
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EAGER 200 Unk Report

Instrument name : Instrument #1 Blind drift (fV): 4
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-01-14 11:23:26 Printed : 08-01-2014 11:33:29
 Sample Ident. : 16 HZ-21 Filename : 288816
 Sample Weight : 2.171 Calc.method: using 'K. Factors'

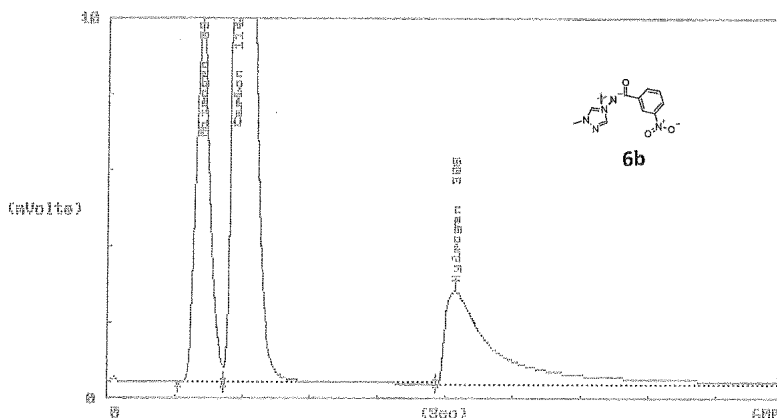
Pk. (#)	Ret Time (Sec)	Area (fV*Sec)	Element % (%)	Area Ratio	Name
1	83	130375	28.617	.485002E+01	Nitrogen
2	113	632321	48.531	.100000E+01	Carbon
3	308	124802	3.419	.506661E+01	Hydrogen





EAGER 200 Stripchart

Sample Ident. : 17 HZ-22 Filename : 288817
 Analysed : 08-01-14 11:33:29 Printed : 08-01-2014 11:43:32



EAGER 200 Peak Integration Report

Instrument name : Instrument #1 Blind drift (fV): 1.7
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-01-14 11:33:29 Printed : 08-01-2014 11:43:32
 Sample Ident. : 17 HZ-22 Filename : 288817
 Sample Weight : 2.121 Calc.method: using 'K. Factors'

No. (#)	Type	Start (Sec)	End (Sec)	Ret Time (Sec)	Height (fV)	Area (fV*Sec)	Area % (%)	Name
1	FU	63	103	83	9218.1	127729	14.69	Nitrogen
2	FU	103	292	114	40576.1	619958	71.32	Carbon
3	RS	292	598	309	2366.5	121519	13.98	Hydrogen

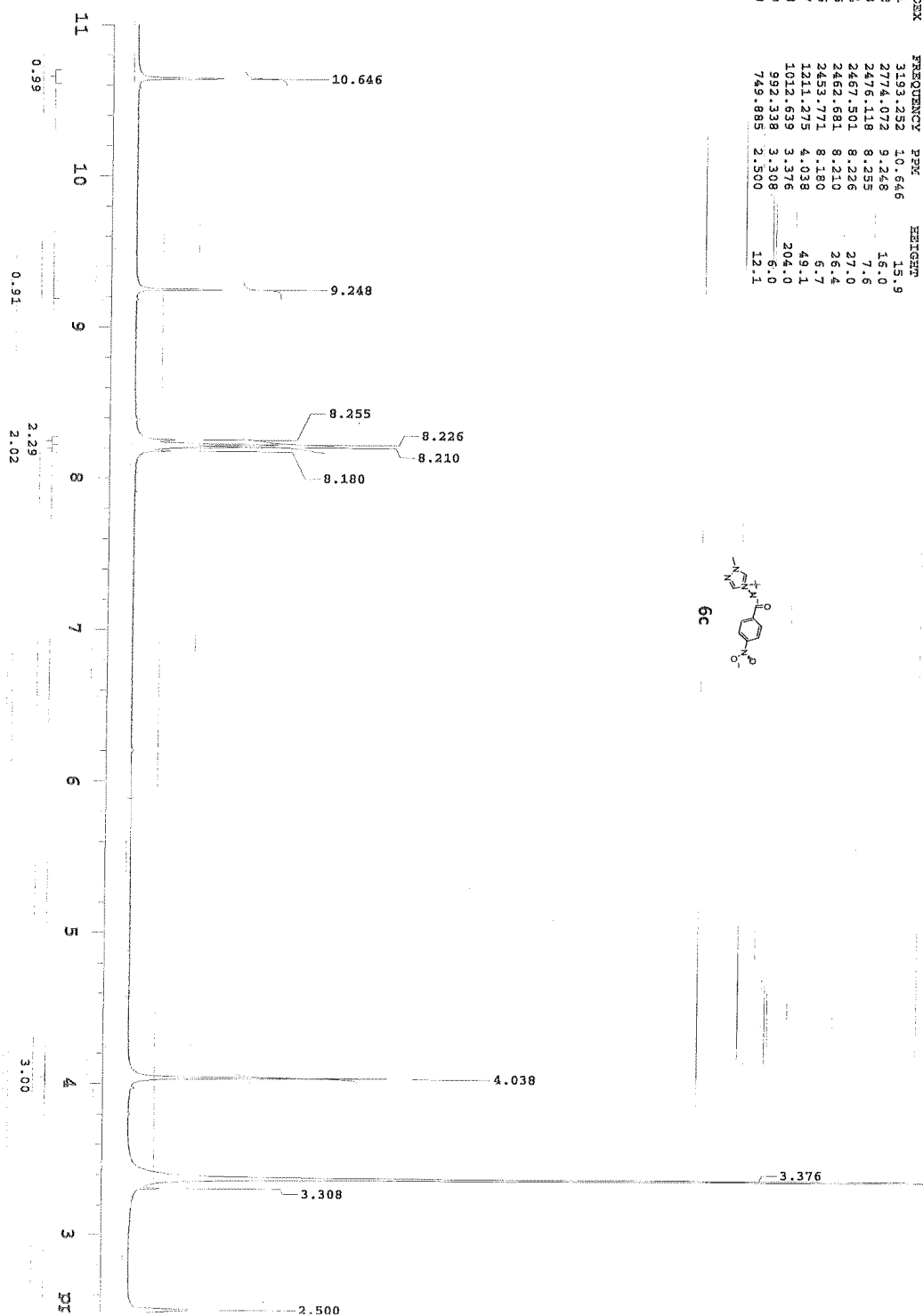
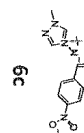
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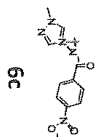
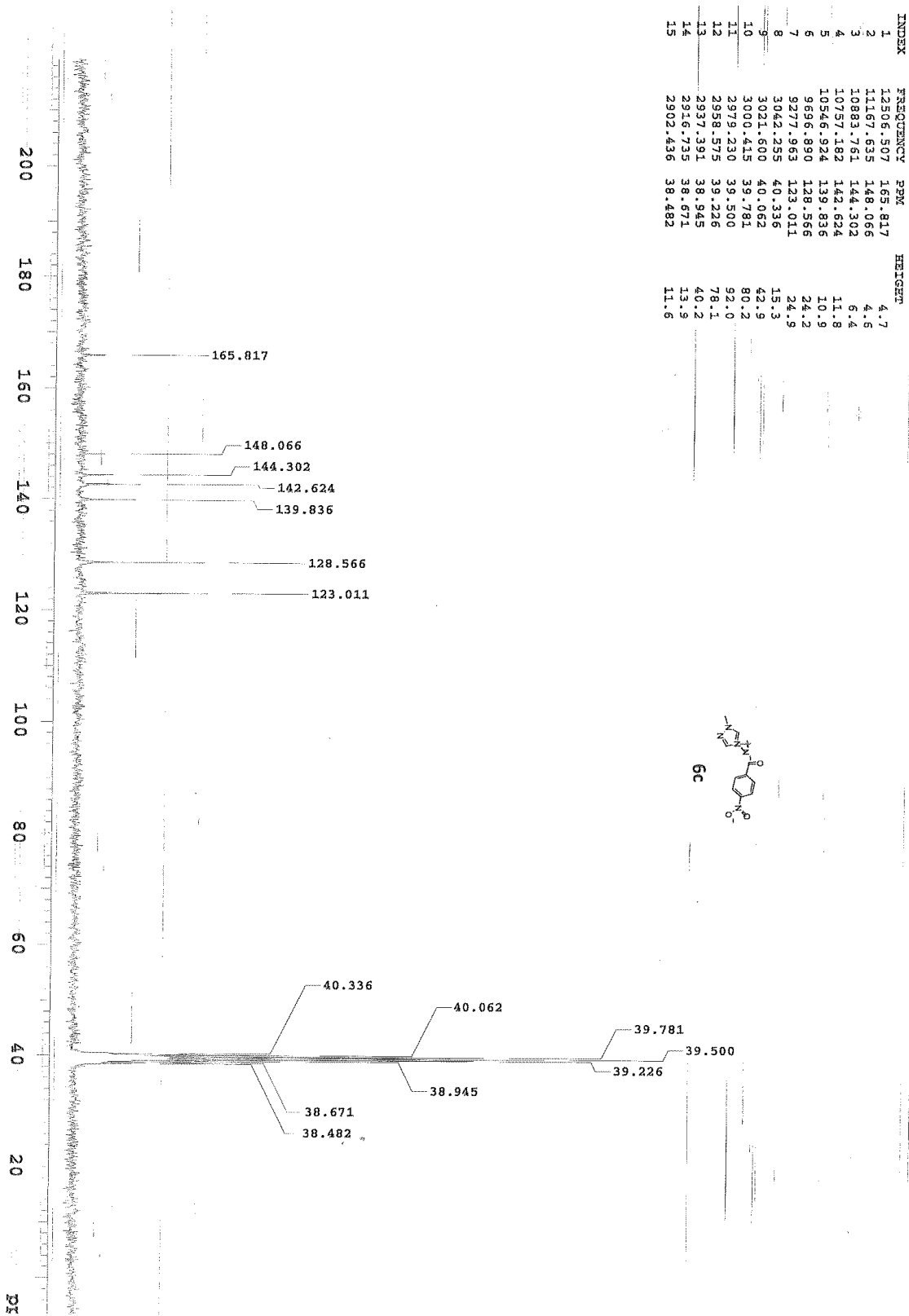
EAGER 200 Unk Report

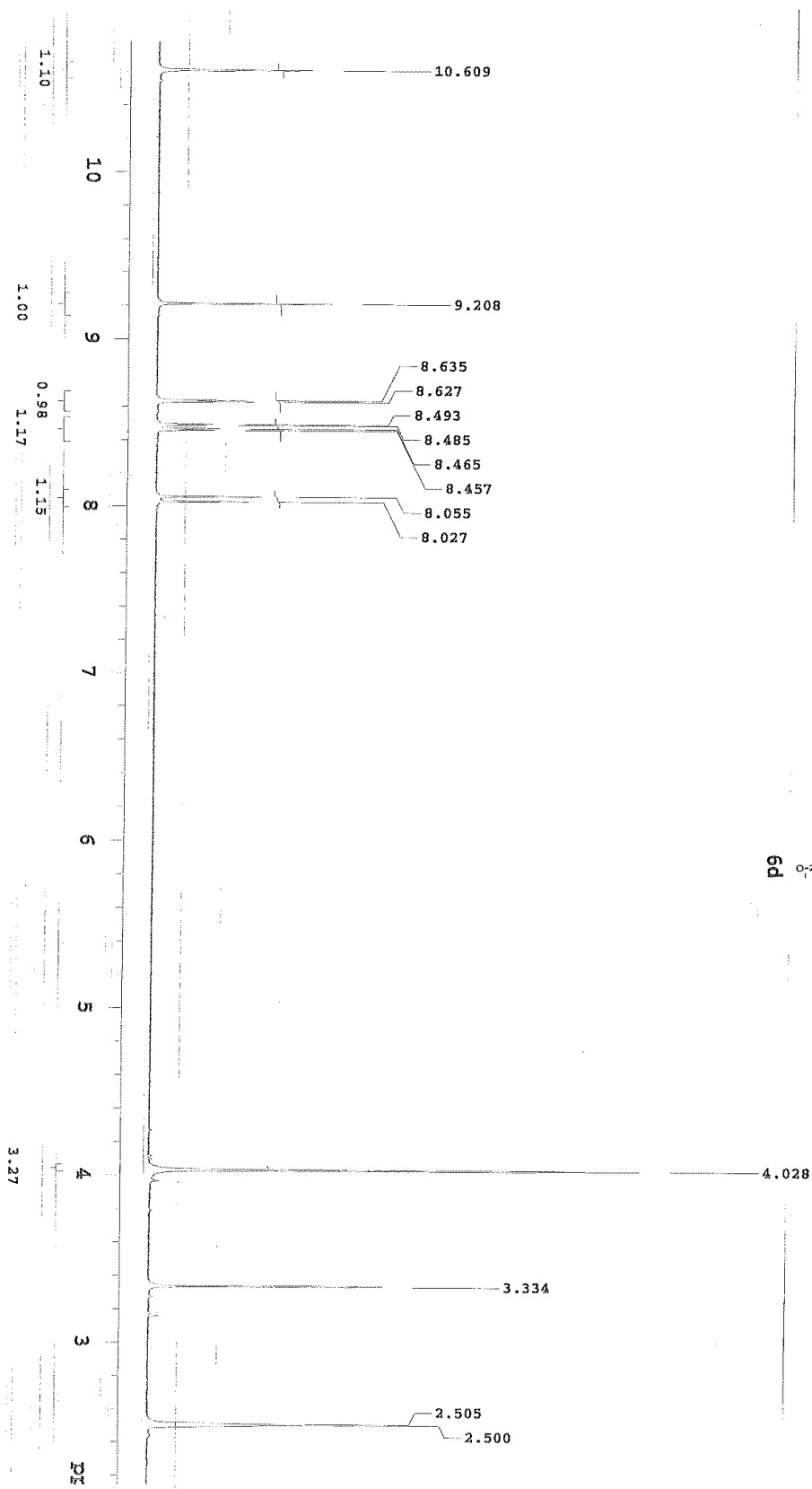
Instrument name : Instrument #1 Blind drift (fV): 1.7
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 08-01-14 11:33:29 Printed : 08-01-2014 11:43:32
 Sample Ident. : 17 HZ-22 Filename : 288817
 Sample Weight : 2.121 Calc.method: using 'K. Factors'

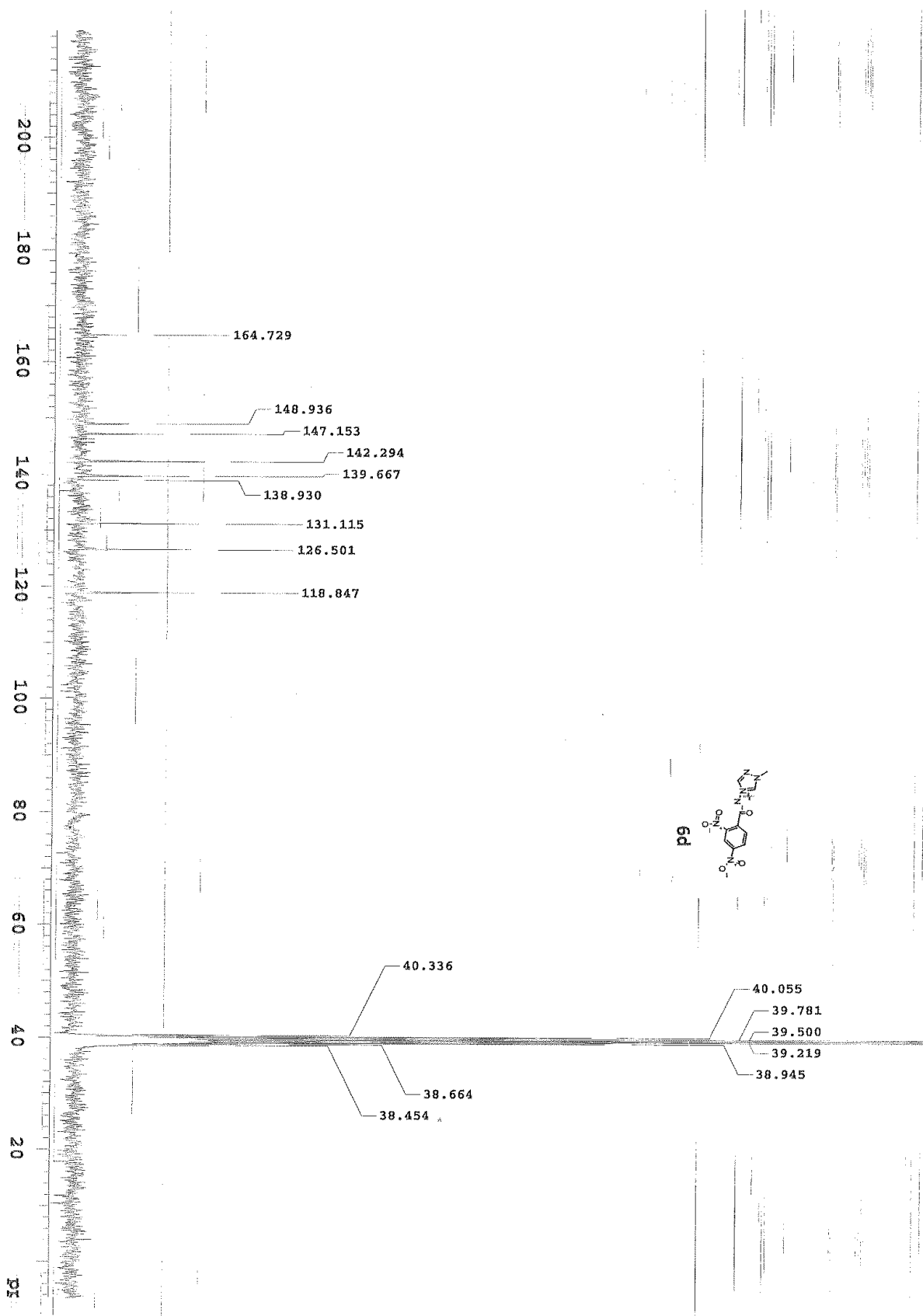
Pk. (#)	Ret Time (Sec)	Area (fV*Sec)	Element % (%)	Area Ratio	Name
1	83	127729	28.696	.485369E+01	Nitrogen
2	114	619958	48.703	.100000E+01	Carbon
3	309	121519	3.408	.510172E+01	Hydrogen

INDEX	FREQUENCY	PPM	HEIGHT
1	3193.252	10.646	15.9
2	2774.072	9.248	16.0
3	2476.118	8.255	7.6
4	2467.501	8.226	27.0
5	2462.681	8.210	26.4
6	2453.771	8.180	6.7
7	1211.275	4.038	49.1
8	1012.639	3.376	204.0
9	992.338	3.308	6.0
10	749.885	2.500	12.1



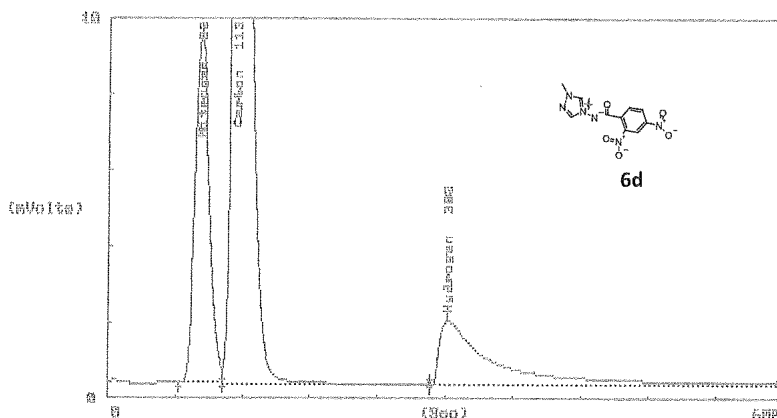






EAGER 200 Stripchart

Sample Ident. : 15 HZ-15 Filename : 288415
 Analysed : 07-24-14 10:07:59 Printed : 07-24-2014 11:49:57



EAGER 200 Peak Integration Report

Instrument name : Instrument #1 Blind drift (fV): 1.5
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 07-24-14 10:07:59 Printed : 07-24-2014 11:49:57
 Sample Ident. : 15 HZ-15 Filename : 288415
 Sample Weight : 2.107 Calc.method: using 'K. Factors'

No. (#)	Type	Start (Sec)	End (Sec)	Ret Time (Sec)	Height (fV)	Area (fV*Sec)	Area % (%)	Name
1	FU	63	102	82	9064.3	125818	17.22	Nitrogen
2	FU	102	287	113	34636.6	516735	70.73	Carbon
3	RS	287	597	302	1638.8	87984	12.04	Hydrogen

730537 100.00

EAGER 200 Unk Report

Instrument name : Instrument #1 Blind drift (fV): 1.5
 Company Name : U of Florida Operator Ident. : KOU
 Analysed : 07-24-14 10:07:59 Printed : 07-24-2014 11:49:57
 Sample Ident. : 15 HZ-15 Filename : 288415
 Sample Weight : 2.107 Calc.method: using 'K. Factors'

Pk. (#)	Ret Time (Sec)	Area (fV*Sec)	Element % (%)	Area Ratio	Name
1	82	125818	28.343	.410700E+01	Nitrogen
2	113	516735	41.471	.100000E+01	Carbon
3	302	87984	2.529	.587306E+01	Hydrogen

INDEX	FREQUENCY	PMN	HEIGHT
1	3212.531	10.710	24.3
2	2803.575	9.347	28.9
3	2708.785	9.031	36.3
4	2706.594	9.023	39.8
5	2658.542	8.863	10.8
6	2656.351	8.856	18.5
7	2654.160	8.849	9.5
8	1218.432	4.062	77.3
9	999.202	3.331	20.1
10	751.638	2.506	14.7
11	749.885	2.500	19.5
12	748.279	2.495	14.5

