

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032216\
 Data File : BF085681.D
 Acq On : 23 Mar 2016 1:48
 Operator : UM/SJ
 Sample : H1864-05
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-9

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.007	236	238	245	rBV	110774	133300	3.03%	0.465%
2	5.430	272	275	277	rBV	1263847	1589541	36.12%	5.542%
3	6.459	363	365	375	rVB	1187064	1035850	23.54%	3.612%
4	6.596	375	377	380	rBV	2657699	2665893	60.59%	9.295%
5	6.824	395	397	400	rBV	565907	747704	16.99%	2.607%
6	6.984	408	411	414	rBV	2490789	2622193	59.59%	9.142%
7	7.396	444	447	450	rBV	1984666	2214306	50.32%	7.720%
8	8.116	508	510	512	rBV	1228827	1062422	24.15%	3.704%
9	9.190	601	604	607	rBV	3114342	4400132	100.00%	15.341%
10	9.865	661	663	666	rVB	1128085	1183427	26.90%	4.126%
11	10.265	694	698	703	rBV5	14194	46203	1.05%	0.161%
12	10.665	729	733	735	rBV2	2141778	2969031	67.48%	10.352%
13	11.202	778	780	783	rBV2	18243	44887	1.02%	0.157%
14	11.351	790	793	795	rBV	1461658	1273122	28.93%	4.439%
15	11.876	838	839	841	rBV	71695	91025	2.07%	0.317%
16	12.665	906	908	911	rBV	143223	174969	3.98%	0.610%
17	12.939	929	932	934	rBV	3943878	4107902	93.36%	14.322%
18	13.979	1021	1023	1026	rBV	1030954	992472	22.56%	3.460%
19	15.397	1144	1147	1150	rBV	530172	645360	14.67%	2.250%
20	15.717	1168	1175	1179	rBV2	64602	297354	6.76%	1.037%
21	15.808	1179	1183	1197	rVB	84066	384644	8.74%	1.341%

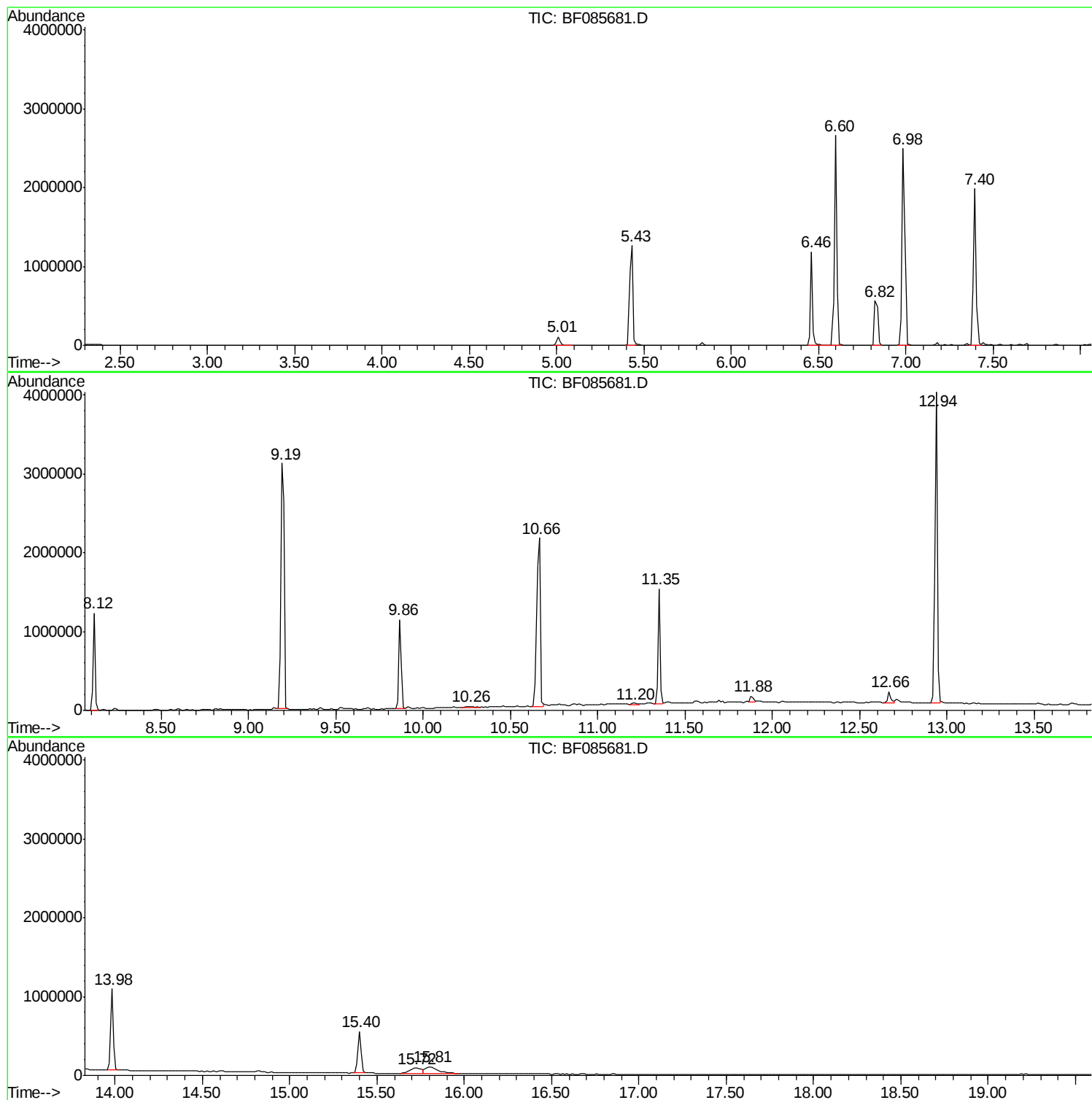
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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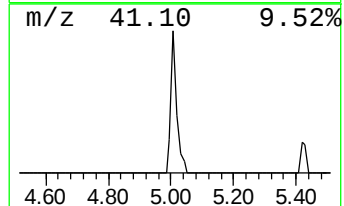
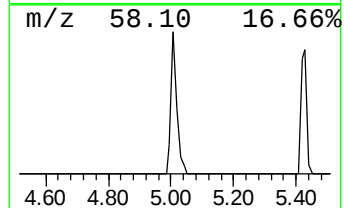
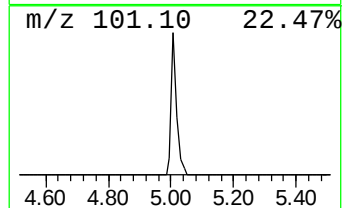
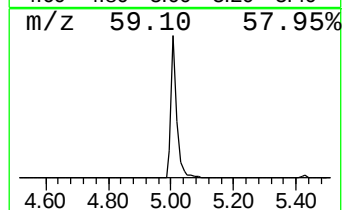
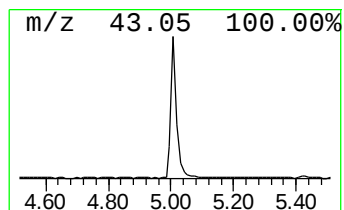
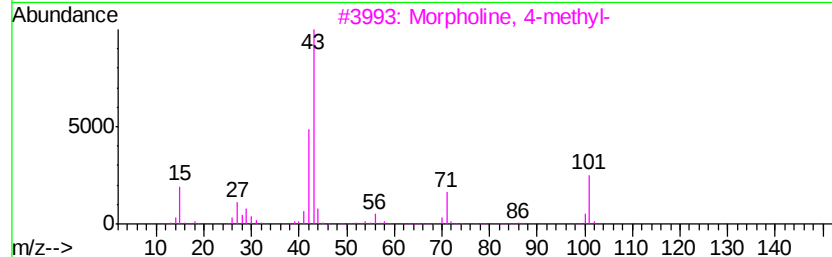
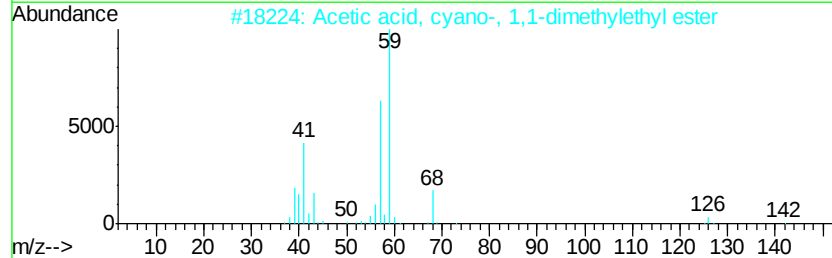
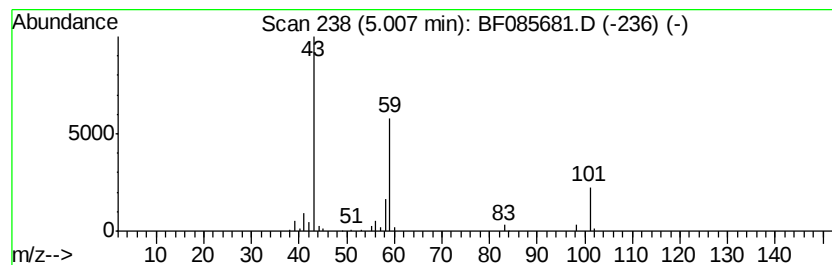
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.01	3.57 ng	133300	1,4-Dichlorobenzene-d4	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9



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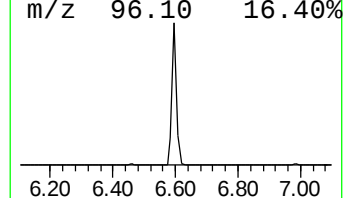
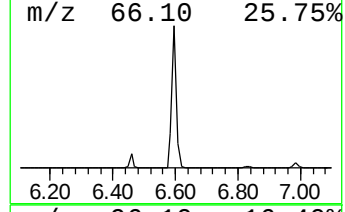
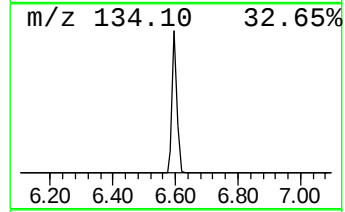
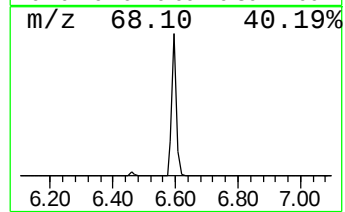
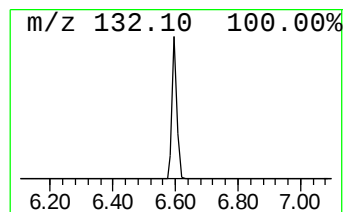
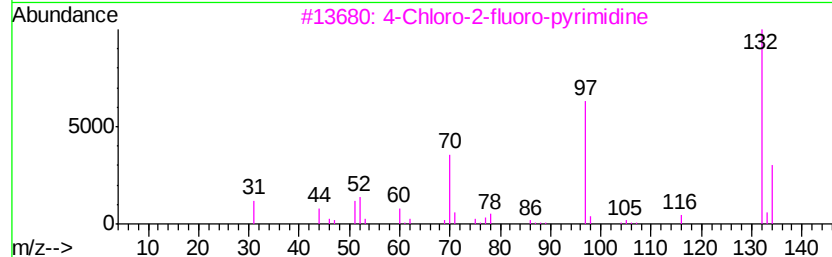
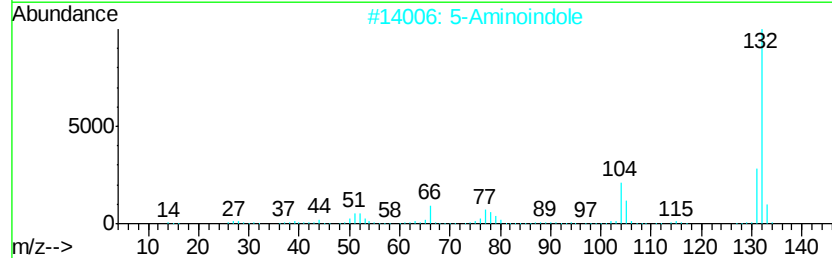
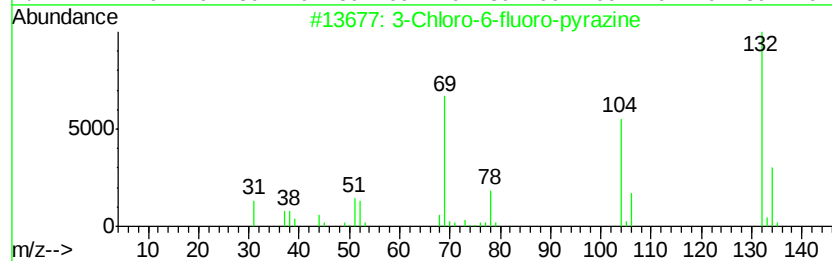
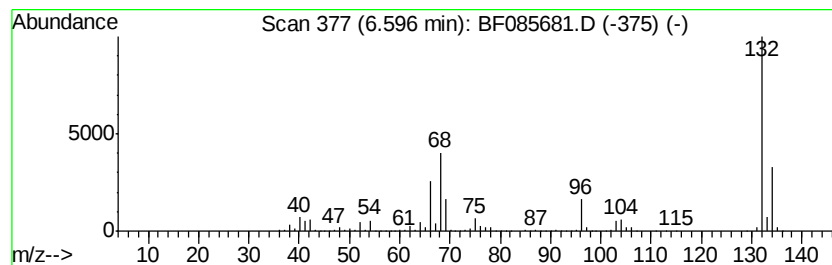
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Peak Number 2 unknown6.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.60	71.31 ng	2665890	1,4-Dichlorobenzene-d4	6.84

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5-Aminoindole	132	C8H8N2	005192-03-0	12
3	4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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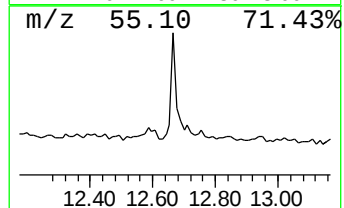
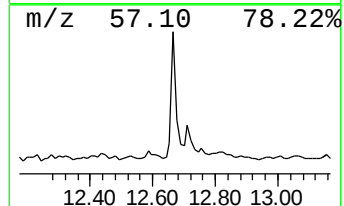
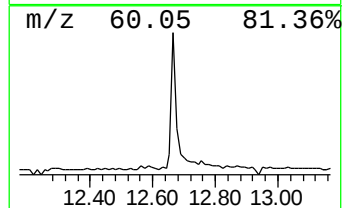
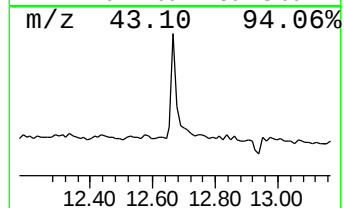
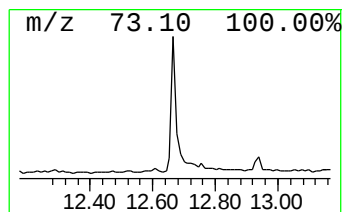
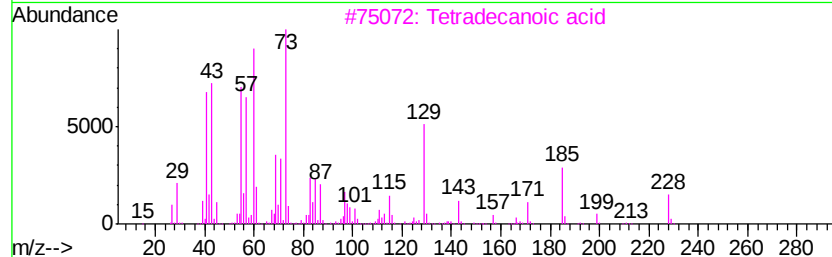
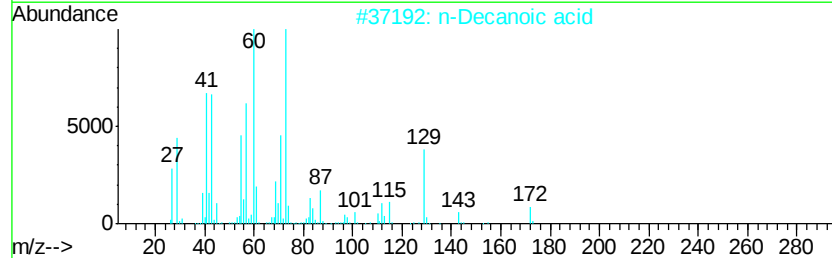
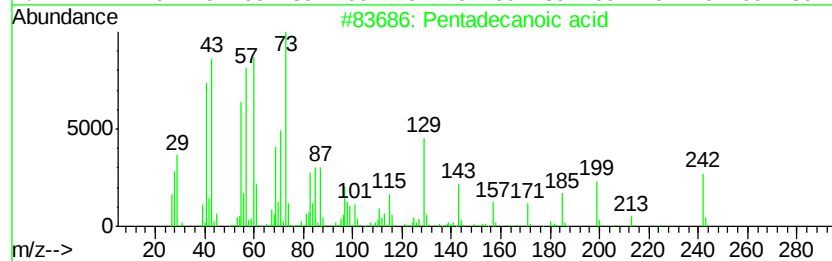
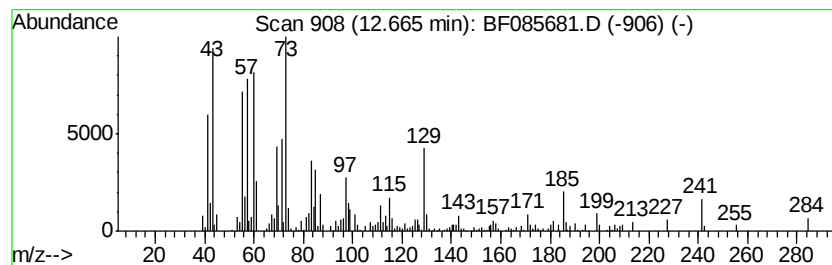
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Peak Number 4 Pentadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
12.67	3.53 ng	174969	Chrysene-d12		13.98
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
2	n-Decanoic acid	172	C10H20O2	000334-48-5	70
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Undecanoic acid	186	C11H22O2	000112-37-8	45
5	Nonanoic acid	158	C9H18O2	000112-05-0	30



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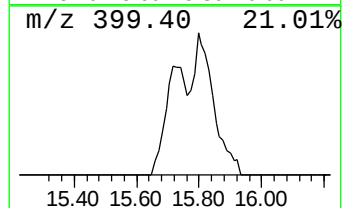
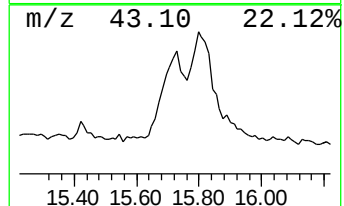
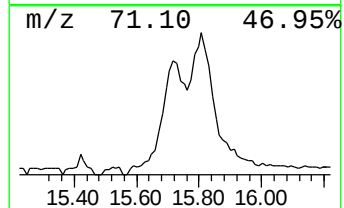
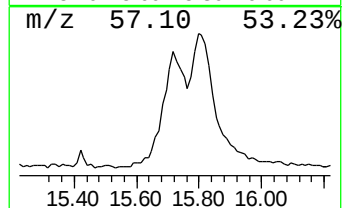
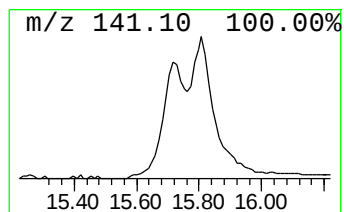
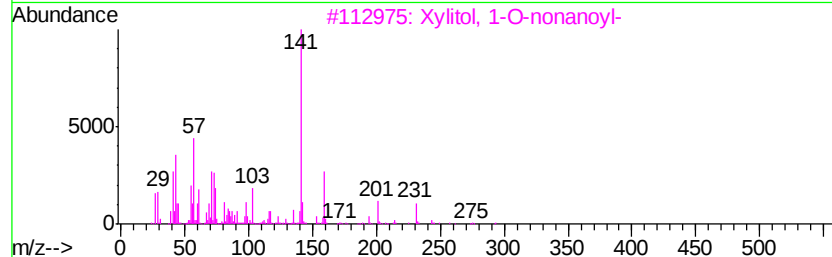
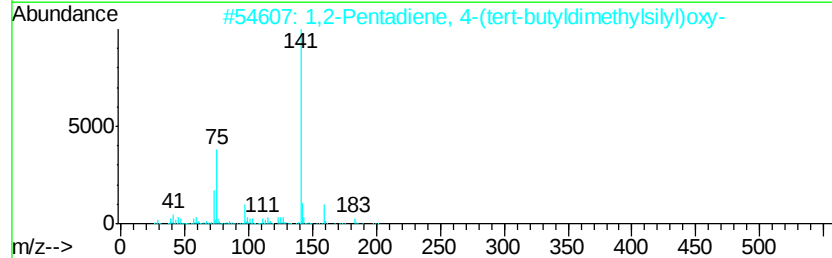
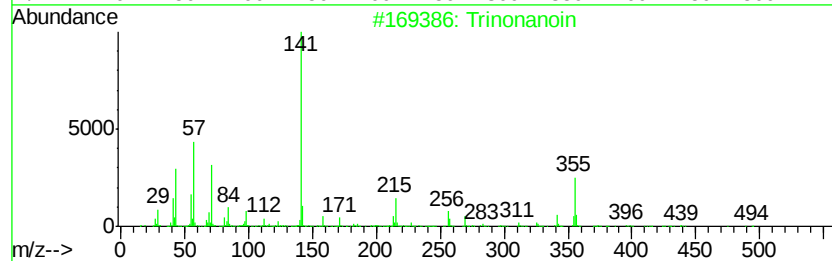
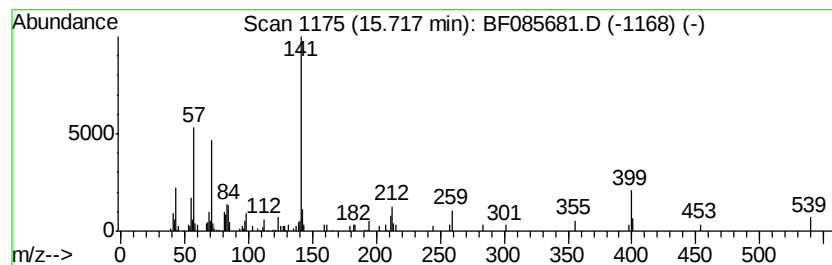
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown15.72 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.72	9.22 ng	297354	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trinonanoic	512	C30H56O6	000126-53-4	37
2		1,2-Pentadiene, 4-(tert-butyldim...	198	C11H22OSi	1000156-17-3	27
3		Xylitol, 1-O-nonanoyl-	292	C14H28O6	1000155-78-2	25
4		2-Fluorobenzoic acid. heptadecyl...	378	C24H39FO2	1000282-96-6	25
5		Diethyl 1,2-cyclopropanedicarbox...	186	C9H14O4	020561-09-5	16



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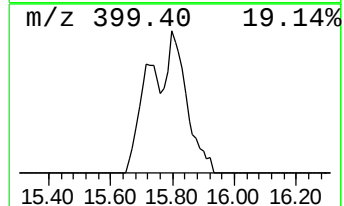
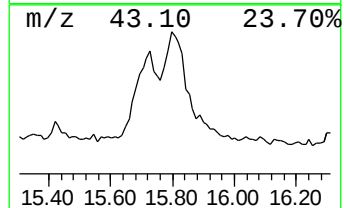
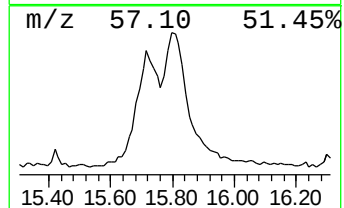
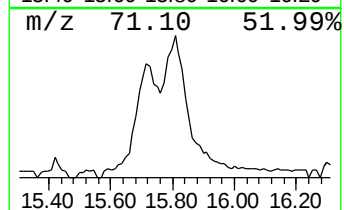
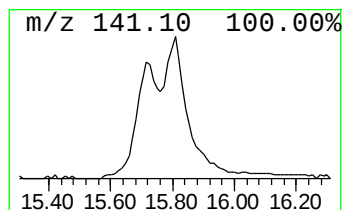
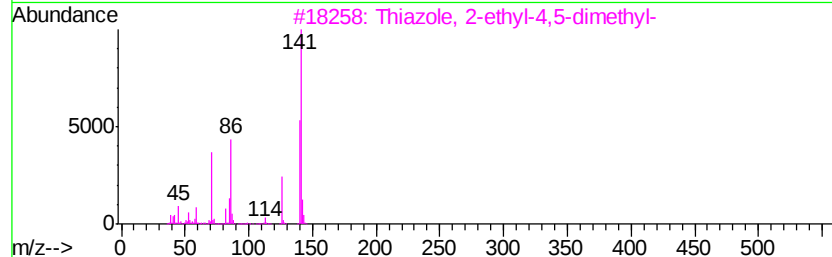
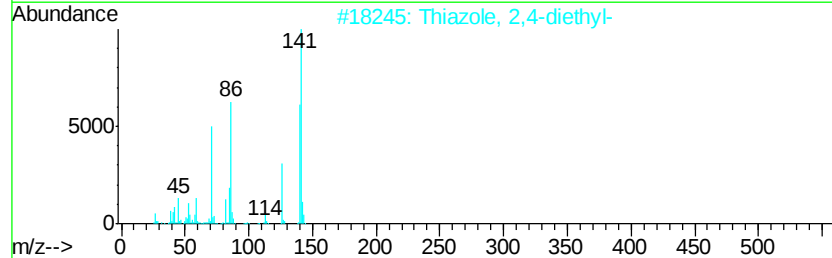
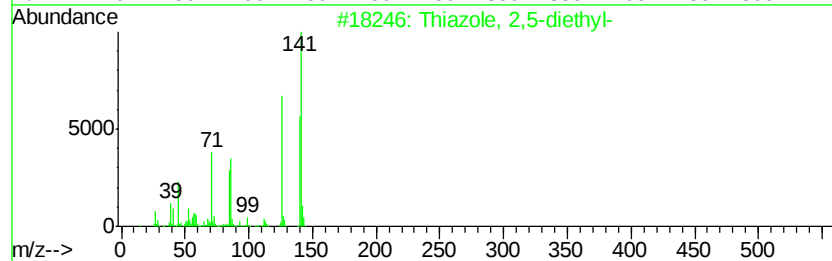
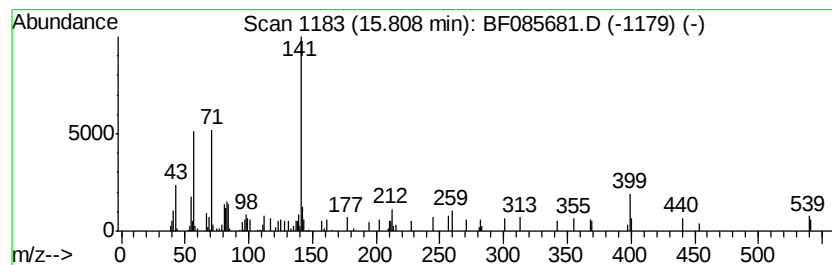
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Peak Number 6 Thiazole, 2,5-diethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.81	11.92 ng	384644	Perylene-d12	15.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thiazole, 2,5-diethyl-	141	C7H11NS	015729-76-7	50
2		Thiazole, 2,4-diethyl-	141	C7H11NS	032272-49-4	50
3		Thiazole, 2-ethyl-4,5-dimethyl-	141	C7H11NS	000873-64-3	40
4		Trinonanoic	512	C30H56O6	000126-53-4	40
5		Methyl 8-oxo-cis-2-nonenate	184	C10H16O3	028297-04-3	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.01	3.6	ng	133300	1	6.84	747704	20.0
unknown6.60	6.60	71.3	ng	2665890	1	6.84	747704	20.0
Pentadecanoic acid	12.67	3.5	ng	174969	5	13.98	992472	20.0
unknown15.72	15.72	9.2	ng	297354	6	15.40	645360	20.0
Thiazole, 2,5-die...	15.81	11.9	ng	384644	6	15.40	645360	20.0