

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF072821\
 Data File : BF124836.D
 Acq On : 28 Jul 2021 19:54
 Operator : JU/CG
 Sample : M3186-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 AREA-3-(0-9)

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF124836.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.140	5	9	13	rBB	11057	12857	6.73%	1.098%
2	5.098	509	512	515	rBB	2022	2478	1.30%	0.212%
3	5.487	574	578	581	rBB	150937	137842	72.14%	11.773%
4	6.498	745	750	753	rBB	141928	140883	73.73%	12.033%
5	6.869	810	813	816	rBB	40071	29676	15.53%	2.535%
6	7.434	905	909	912	rBB	114700	95013	49.73%	8.115%
7	8.051	1011	1014	1018	rBV	25565	17718	9.27%	1.513%
8	8.151	1028	1031	1034	rBB	54452	41904	21.93%	3.579%
9	9.228	1210	1214	1217	rBV	237916	191069	100.00%	16.319%
10	9.910	1326	1330	1333	rBB	57850	51142	26.77%	4.368%
11	10.698	1460	1464	1467	rBB	148267	119217	62.39%	10.182%
12	11.398	1579	1583	1585	rBV	58538	51870	27.15%	4.430%
13	11.916	1669	1671	1673	rBB	11267	7442	3.89%	0.636%
14	12.604	1786	1788	1791	rBB	4461	3050	1.60%	0.261%
15	12.833	1825	1827	1830	rBB	6650	5162	2.70%	0.441%
16	12.980	1848	1852	1855	rBV	198202	183055	95.81%	15.635%
17	13.886	2002	2006	2015	rBB2	5872	11081	5.80%	0.946%
18	14.033	2027	2031	2034	rBV	38641	33569	17.57%	2.867%
19	15.074	2205	2208	2211	rBV	2240	2444	1.28%	0.209%
20	15.439	2267	2270	2273	rBB	2296	2298	1.20%	0.196%
21	15.509	2277	2282	2286	rBB2	29140	31037	16.24%	2.651%

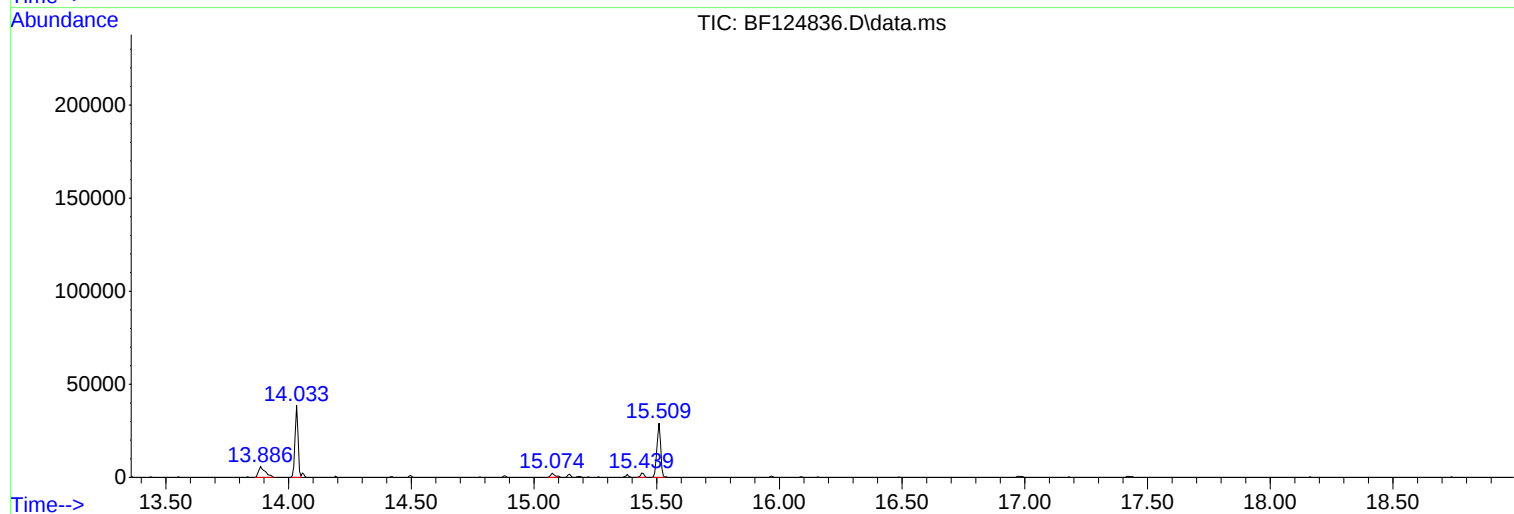
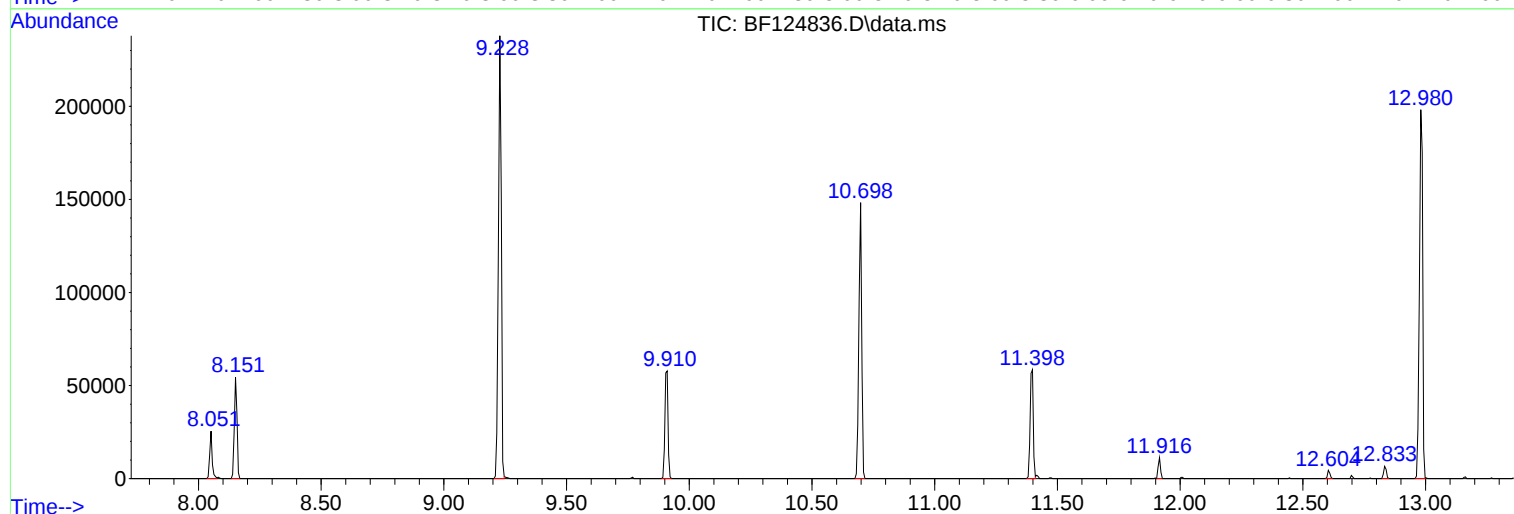
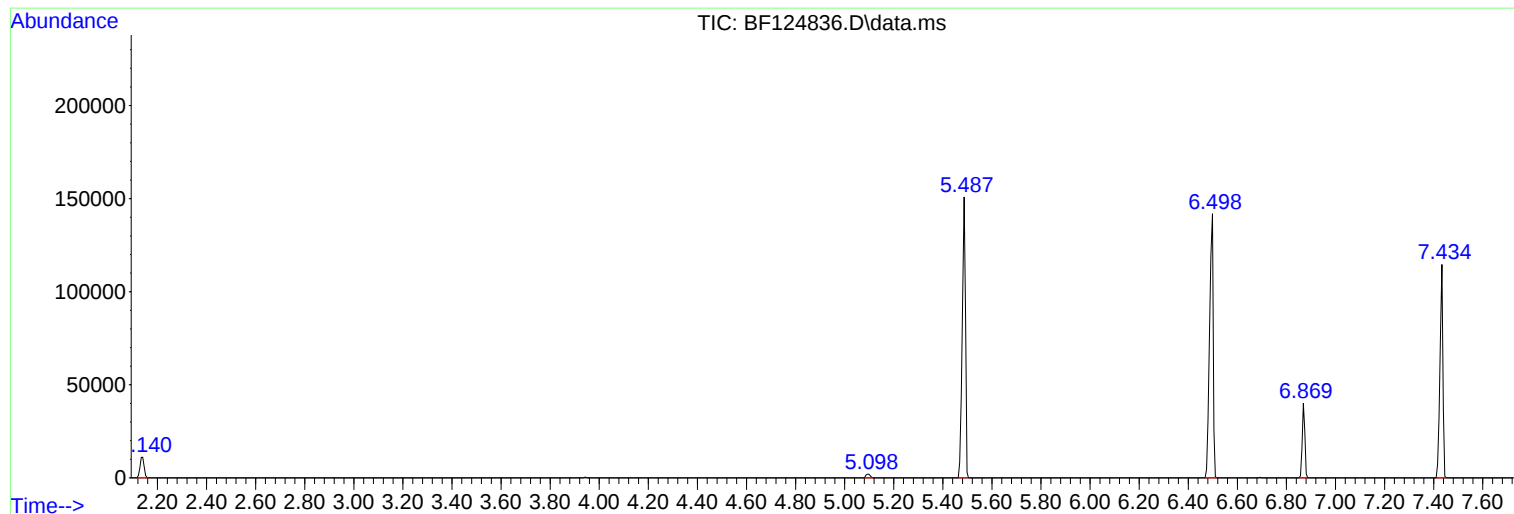
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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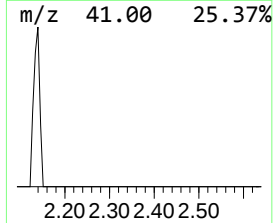
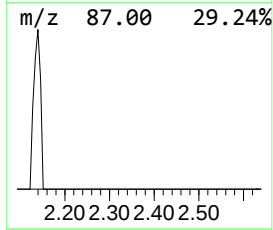
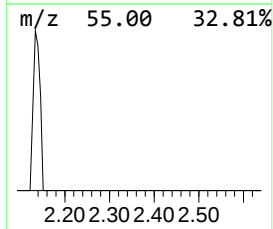
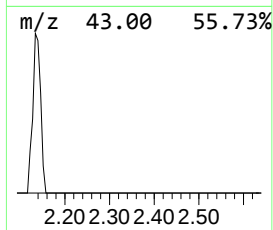
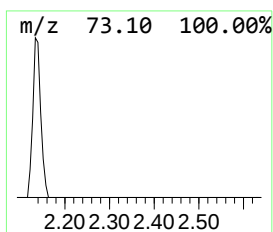
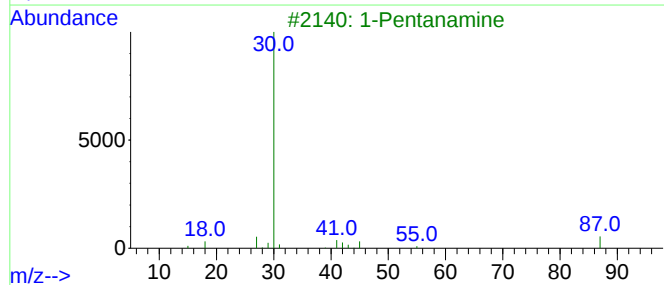
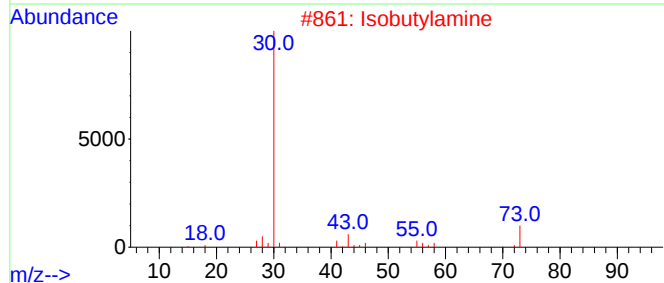
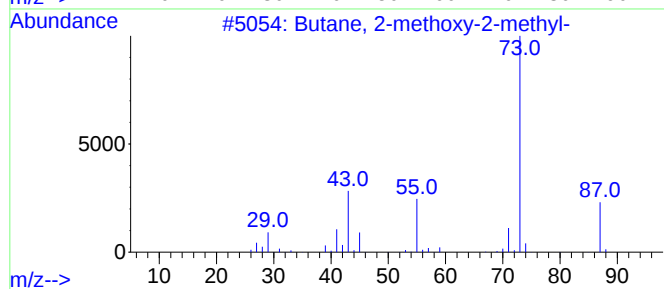
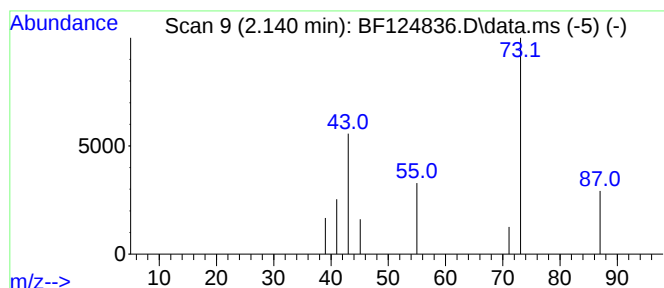
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF072221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown2.140 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.140	8.66 ng	12857	1,4-Dichlorobenzene-d4	6.869

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	9
2			Isobutylamine	73	C4H11N	000078-81-9	7
3			1-Pentanamine	87	C5H13N	000110-58-7	4
4			1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	4
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	4



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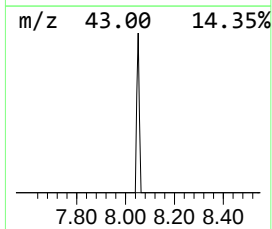
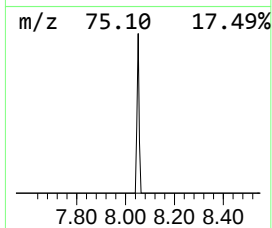
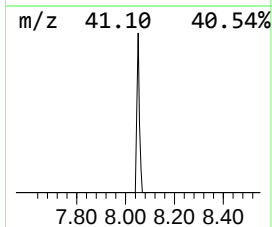
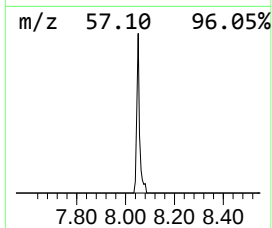
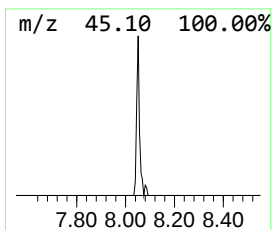
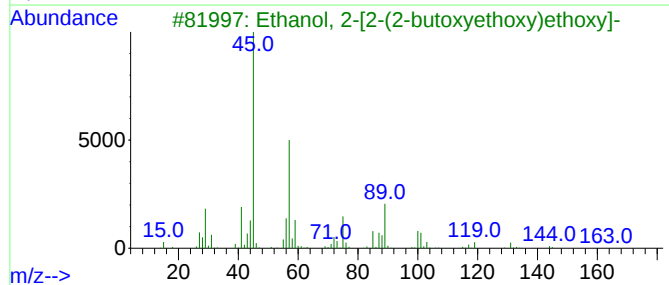
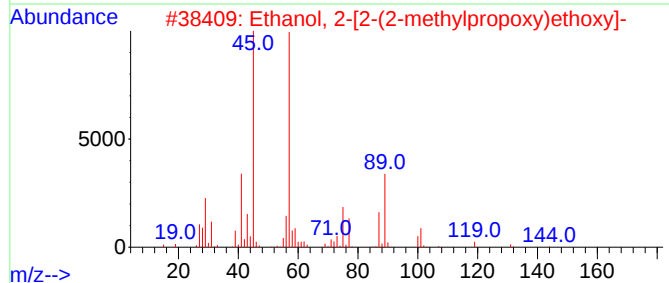
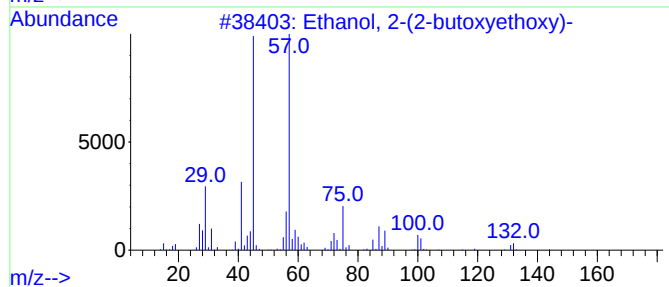
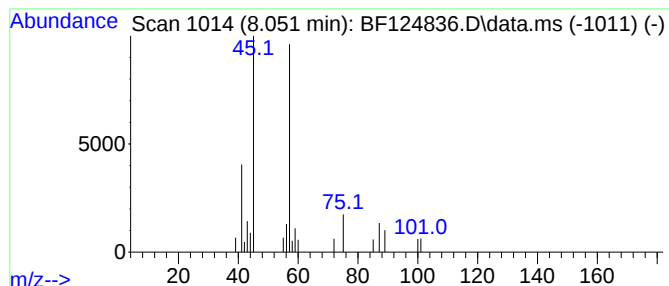
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	8.46 ng	17718	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	42
5			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	39



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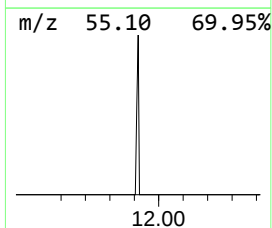
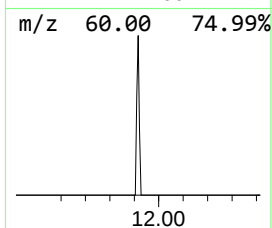
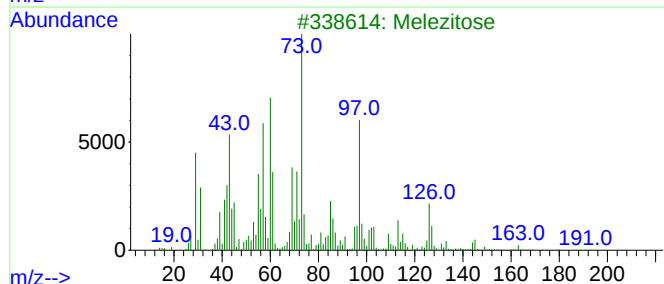
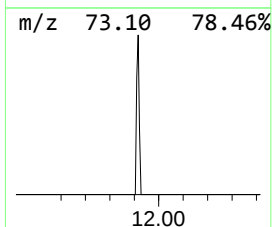
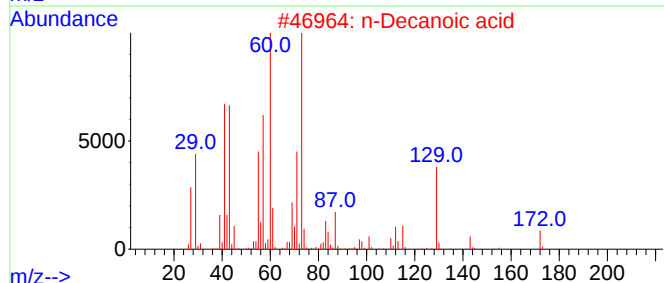
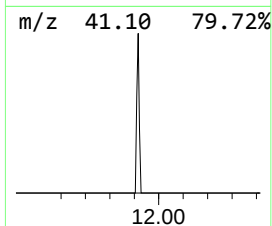
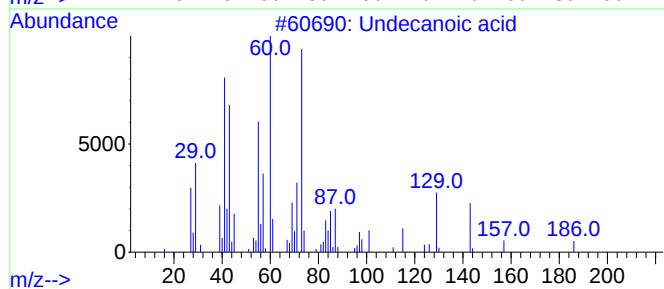
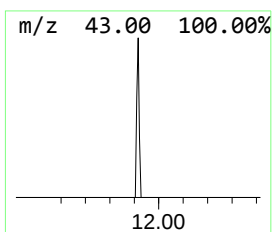
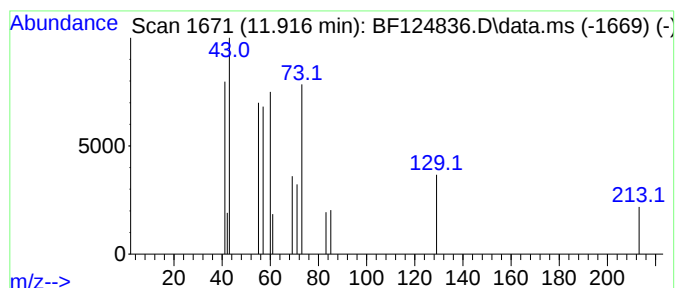
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Peak Number 3 Undecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	2.87 ng	7442	Phenanthrene-d10	11.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	50
2			n-Decanoic acid	172	C10H20O2	000334-48-5	50
3			Melezitose	504	C18H32O16	000597-12-6	42
4			Dodecanoic acid	200	C12H24O2	000143-07-7	42
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	40



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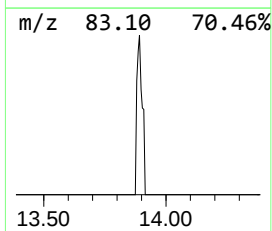
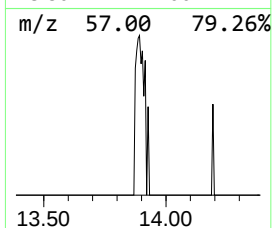
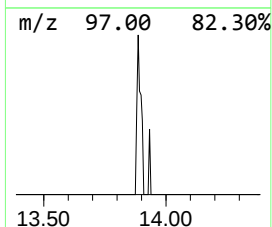
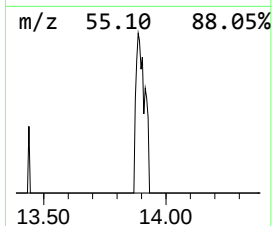
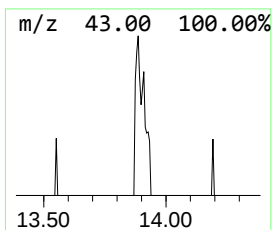
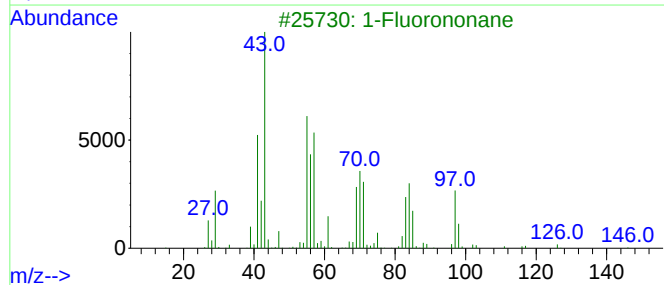
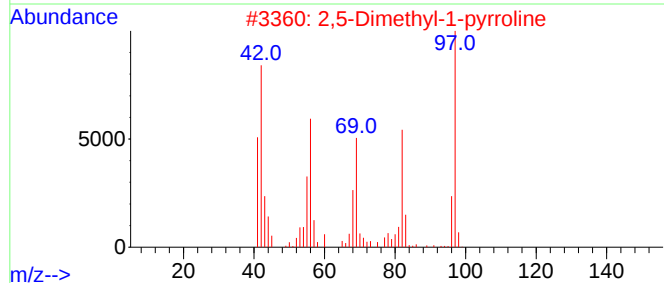
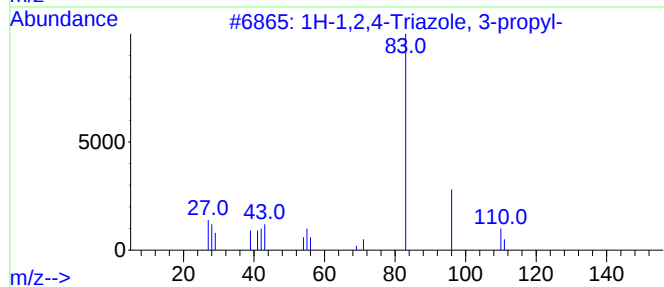
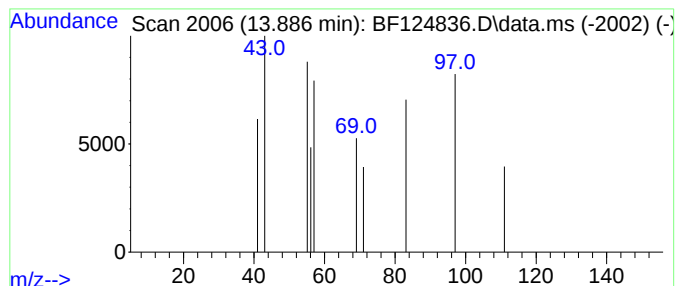
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Peak Number 4 unknown13.886 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	6.60 ng	11081	Chrysene-d12	14.033

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-1,2,4-Triazole, 3-propyl-		111	C5H9N3		019932-60-6	17
2	2,5-Dimethyl-1-pyrroline		97	C6H11N		000822-64-0	9
3	1-Fluorononane		146	C9H19F		000463-18-3	9
4	6-Methyloctyl acetate		186	C11H22O2		1000439-66-5	9
5	(S)-(+)-6-Methyl-1-octanol		144	C9H20O		110453-78-6	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethanol, 2-(2-b...	8.051	8.5	ng	17718	2	8.151	41904	20.0
Undecanoic acid	11.916	2.9	ng	7442	4	11.398	51870	20.0
unknown13.886	13.886	6.6	ng	11081	5	14.033	33569	20.0