

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\
 Data File : BM010188.D
 Acq On : 24 May 2017 19:38
 Operator : SJ/MA
 Sample : I3305-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 DSK-SB1(5-10)

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_M\METHODS\8270-BM051917.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	5.069	333	337	346	rVB	244620	341791	2.64%	0.535%
2	5.534	409	416	430	rBV	3577321	5014926	38.76%	7.856%
3	7.139	681	689	704	rBV	3124352	4997314	38.63%	7.828%
4	7.492	741	749	760	rBV	3397683	5325732	41.17%	8.342%
5	7.951	819	827	832	rBV	539547	882200	6.82%	1.382%
6	8.269	874	881	891	rBV	2633892	4219554	32.62%	6.610%
7	9.139	1020	1029	1037	rBV	1839707	2984260	23.07%	4.675%
8	10.757	1296	1304	1311	rBV	623423	1060817	8.20%	1.662%
9	13.204	1713	1720	1728	rVB	5203696	7435177	57.47%	11.647%
10	14.039	1857	1862	1870	rBV	575425	803193	6.21%	1.258%
11	14.580	1948	1954	1964	rVB2	904276	1438555	11.12%	2.253%
12	16.074	2201	2208	2218	rBV	4614109	6202727	47.94%	9.716%
13	17.327	2414	2421	2429	rBV	1333578	1830433	14.15%	2.867%
14	18.174	2560	2565	2576	rBV2	302887	440487	3.40%	0.690%
15	19.445	2777	2781	2785	rBV2	119047	163514	1.26%	0.256%
16	19.927	2858	2863	2870	rBV	10630661	12937223	100.00%	20.265%
17	21.150	3068	3071	3078	rBV7	114374	241614	1.87%	0.378%
18	21.486	3123	3128	3135	rBV	2263334	2733105	21.13%	4.281%
19	22.527	3301	3305	3315	rBV	1214511	1723609	13.32%	2.700%
20	23.850	3523	3530	3539	rVB	1521871	3063140	23.68%	4.798%

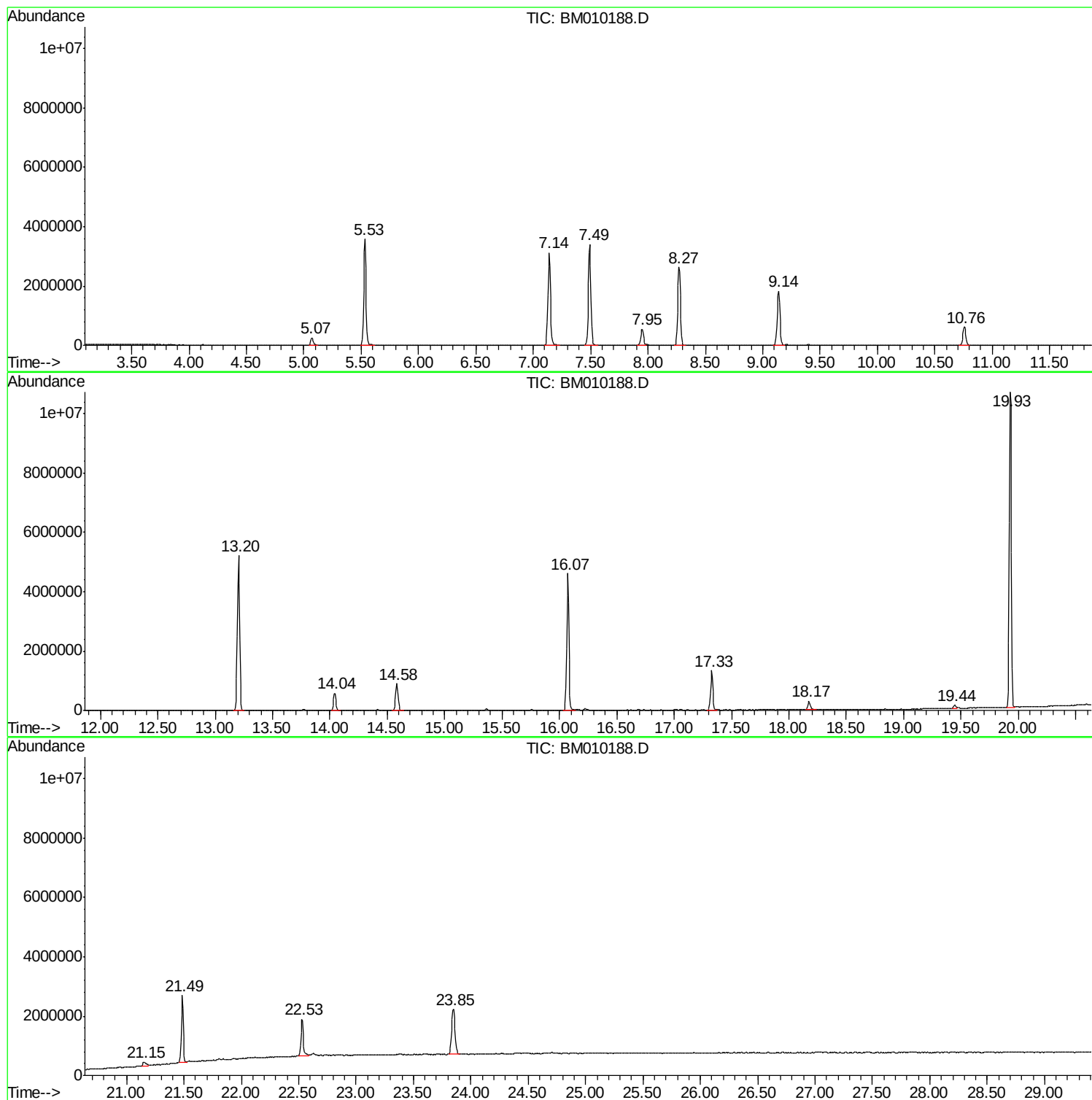
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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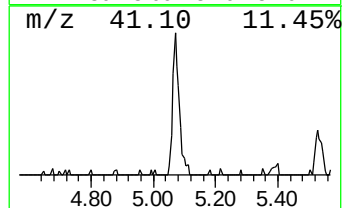
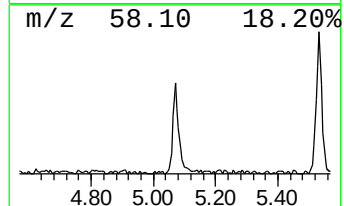
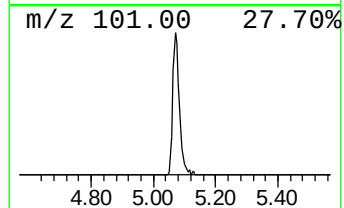
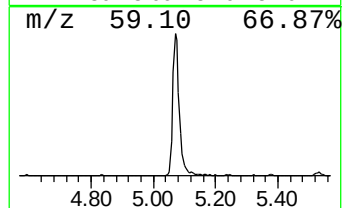
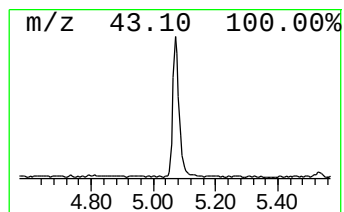
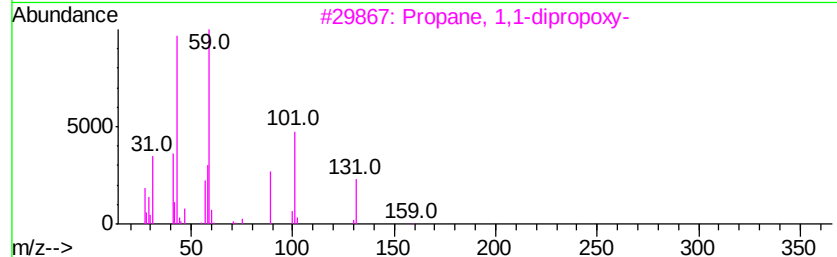
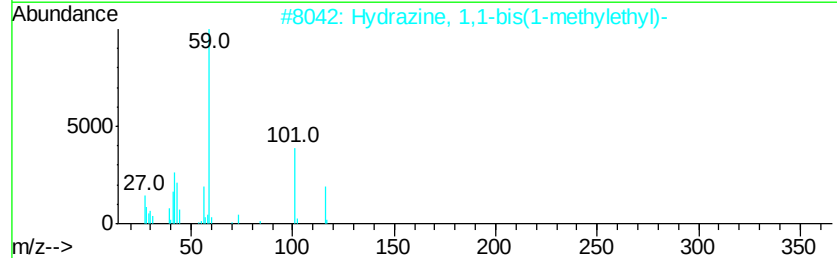
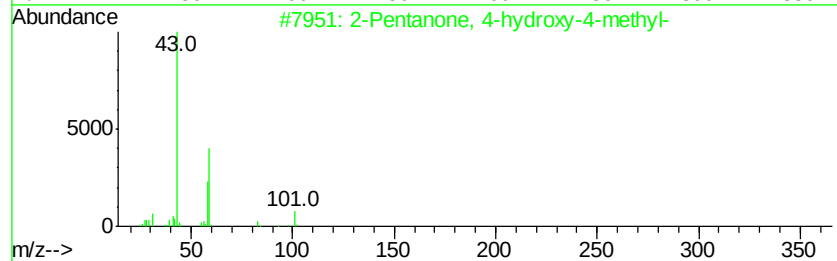
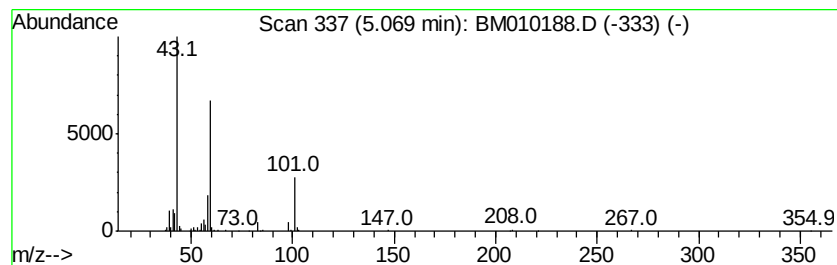
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	7.75 ng	341791	1,4-Dichlorobenzene-d4	7.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	50
3			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	38
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	37
5			Dimethadione	129	C5H7NO3	000695-53-4	28



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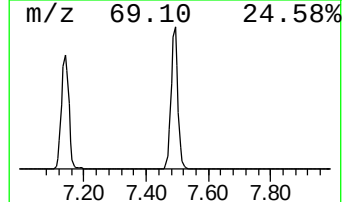
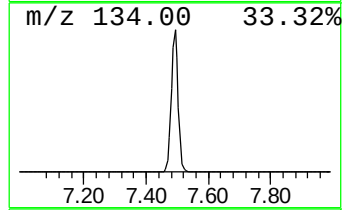
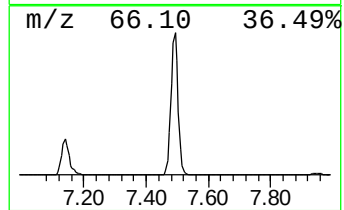
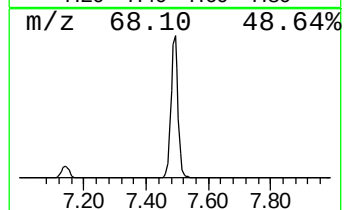
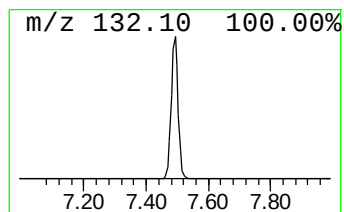
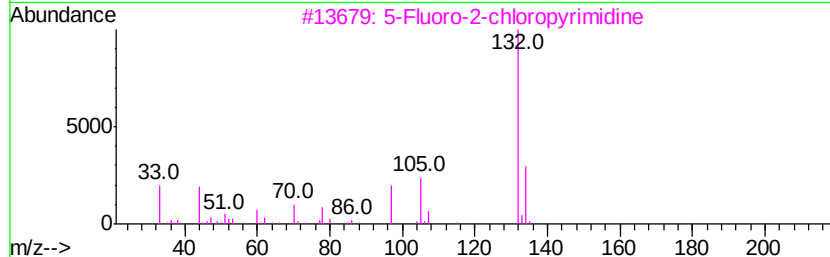
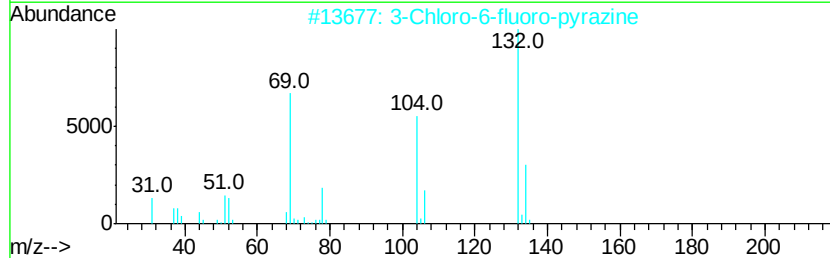
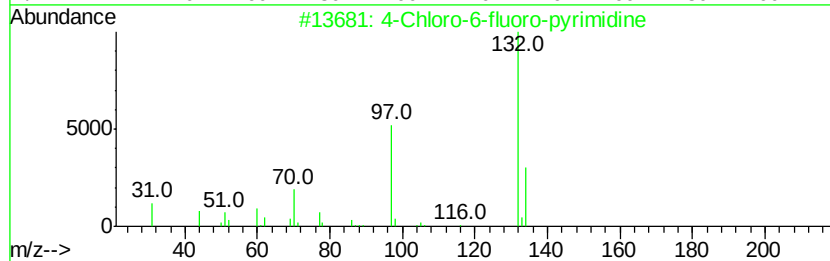
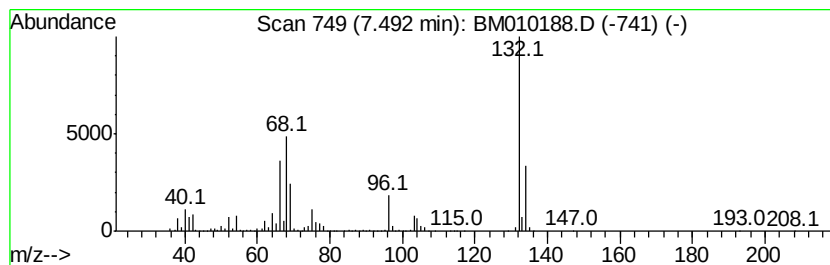
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Peak Number 2 unknown7.49 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.49	120.74 ng	5325730	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	10
5		Benzene, 1-methyl-4-(1-methyleth...	132	C10H12	001195-32-0	10



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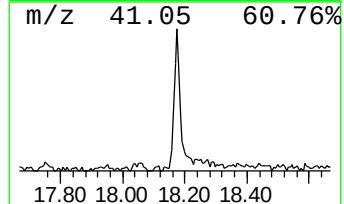
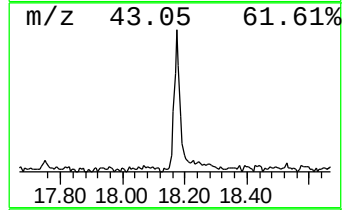
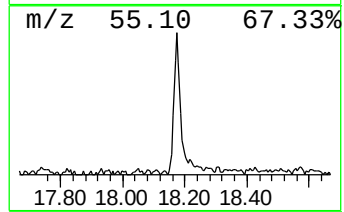
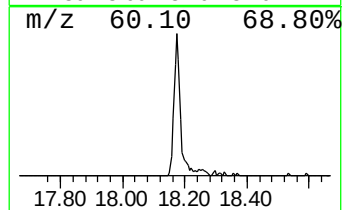
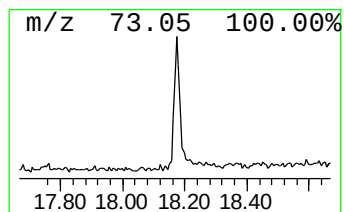
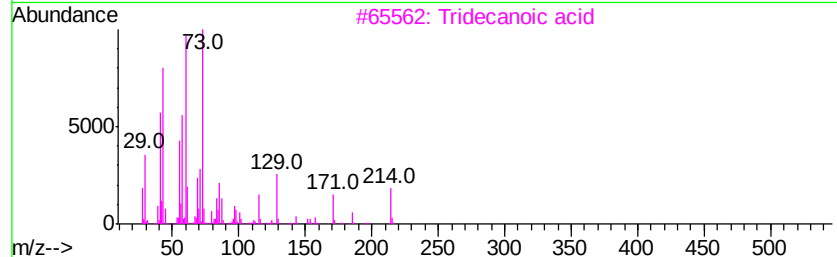
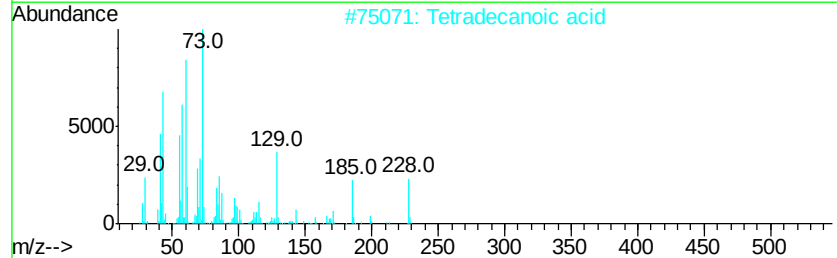
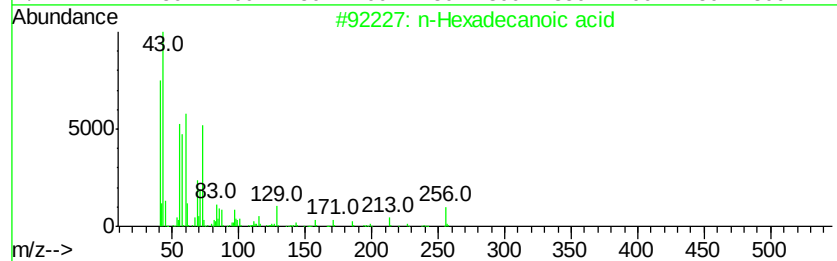
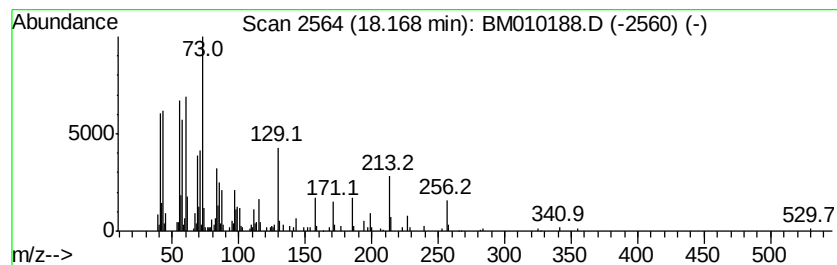
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.17	4.81 ng	440487	Phenanthrene-d10	17.33	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	78
4	Dodecanoic acid	200	C12H24O2	000143-07-7	70
5	Undecanoic acid	186	C11H22O2	000112-37-8	59



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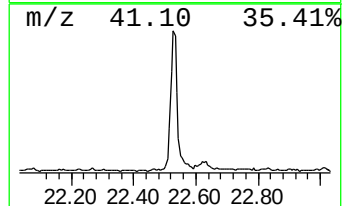
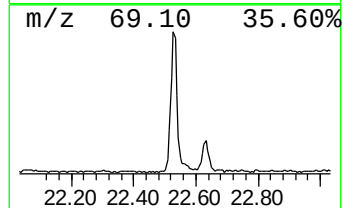
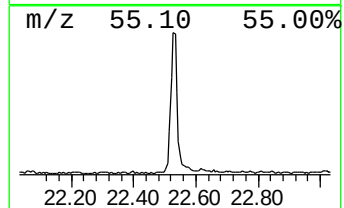
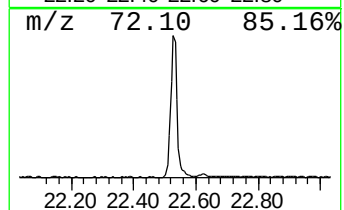
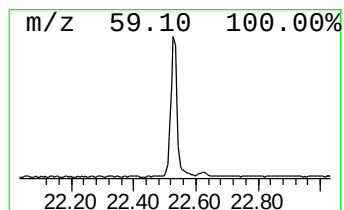
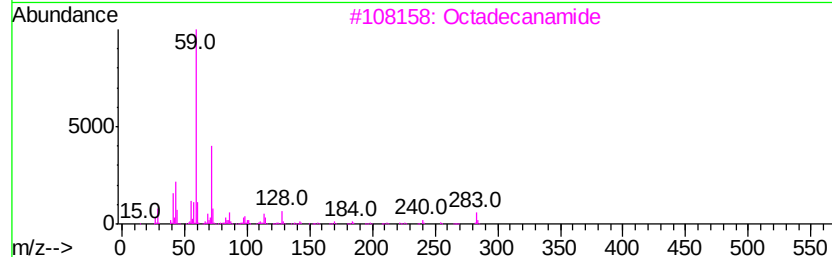
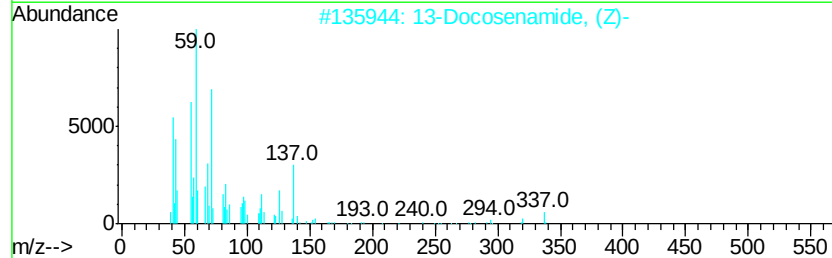
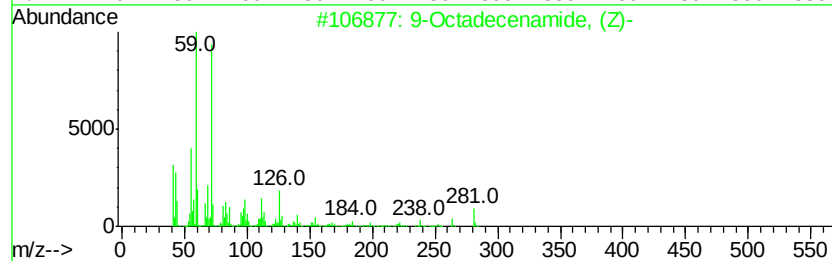
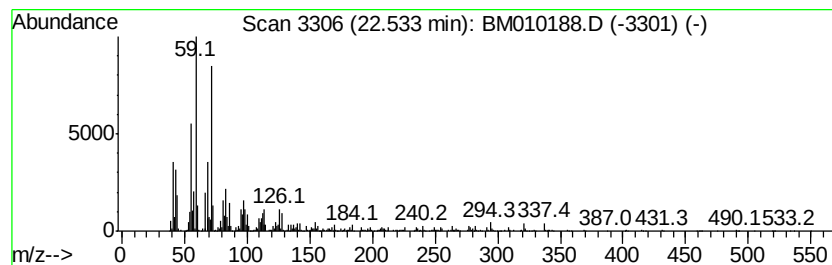
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.53	12.61 ng	1723610	Chrysene-d12	21.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	86
3		Octadecanamide	283	C18H37NO	000124-26-5	38
4		Octanamide	143	C8H17NO	000629-01-6	38
5		Dodecanamide	199	C12H25NO	001120-16-7	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.07	7.8	ng	341791	1	7.95	882200	20.0
unknown7.49	7.49	120.7	ng	5325730	1	7.95	882200	20.0
n-Hexadecanoic acid	18.17	4.8	ng	440487	4	17.33	1830430	20.0
9-Octadecenamide,...	22.53	12.6	ng	1723610	5	21.49	2733110	20.0