

Data Path : Z:\HPCHEM1\BNA M\DATA\BM072617\
 Data File : BM010988.D
 Acq On : 27 Jul 2017 01:36
 Operator : SJ/JU
 Sample : I4400-04
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB02B

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-BM072617.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	4.587	300	306	314	rBV	589408	775072	4.11%	0.700%
2	5.034	375	382	391	rBV	6345097	8737811	46.31%	7.897%
3	6.592	637	647	659	rBV	6411735	9907377	52.51%	8.954%
4	6.934	696	705	713	rBV	6448053	9501634	50.36%	8.587%
5	7.392	776	783	790	rVB	1344071	2011160	10.66%	1.818%
6	7.704	829	836	845	rVB	4706325	7208364	38.21%	6.515%
7	8.539	971	978	987	rBV	4034510	6345524	33.63%	5.735%
8	10.151	1245	1252	1259	rVB	1685044	2662350	14.11%	2.406%
9	12.657	1671	1678	1688	rBV	9710591	14167753	75.09%	12.804%
10	13.515	1819	1824	1834	rVB	778870	1079680	5.72%	0.976%
11	14.045	1908	1914	1922	rBV2	2413335	3662228	19.41%	3.310%
12	15.551	2163	2170	2181	rBV	9237889	12414923	65.80%	11.220%
13	16.803	2377	2383	2391	rBV	3213379	4408876	23.37%	3.985%
14	17.733	2536	2541	2551	rBV	650369	868227	4.60%	0.785%
15	19.033	2757	2762	2769	rBV2	530734	691438	3.66%	0.625%
16	19.468	2830	2836	2842	rBV	15925508	18867281	100.00%	17.052%
17	20.768	3053	3057	3065	rBV5	181559	322339	1.71%	0.291%
18	21.021	3095	3100	3106	rBV	3386443	4141075	21.95%	3.743%
19	23.138	3454	3460	3466	rVB	1669168	2873702	15.23%	2.597%

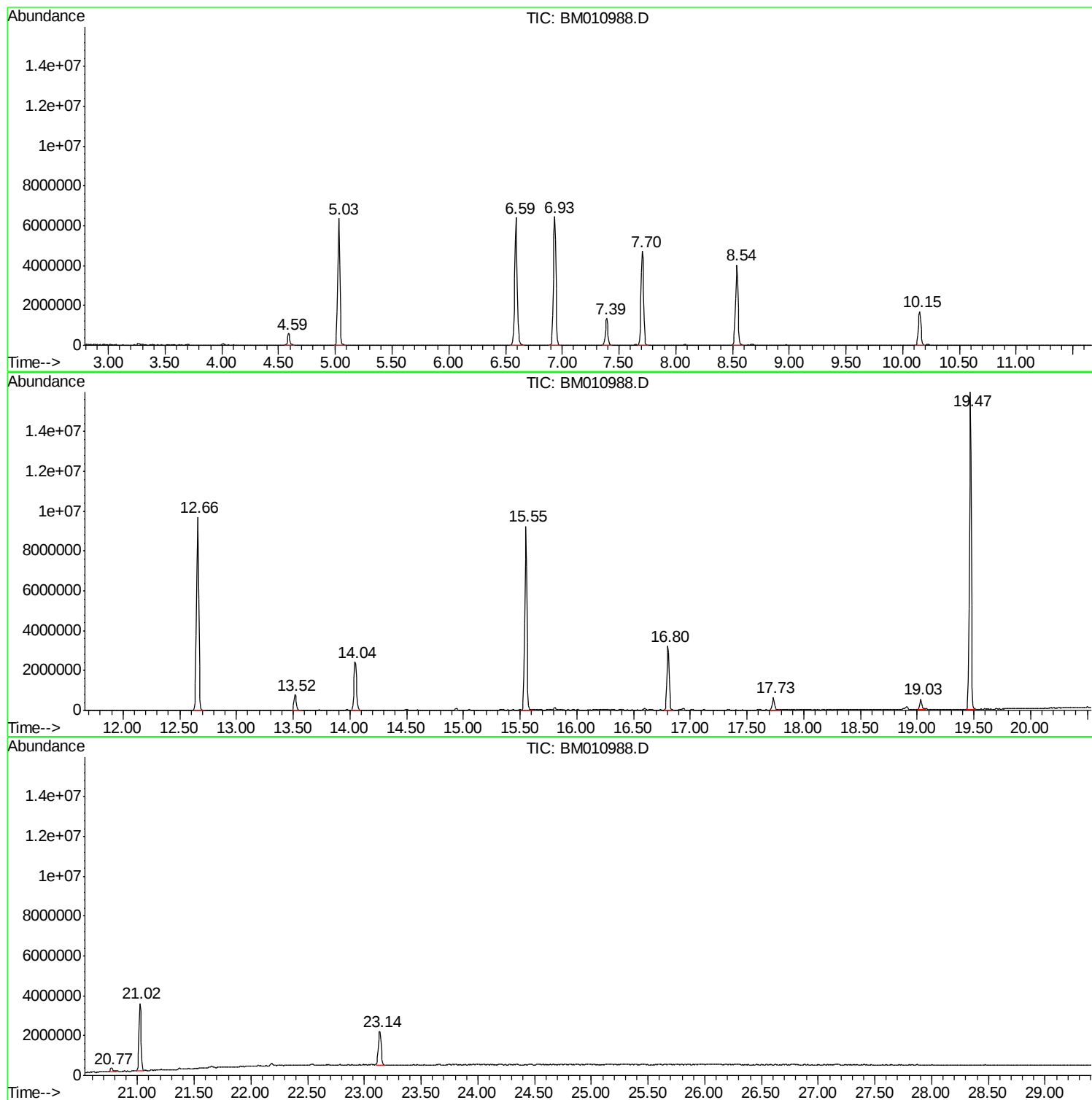
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM072617.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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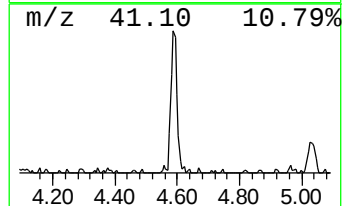
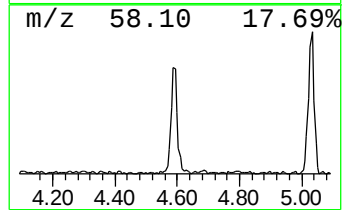
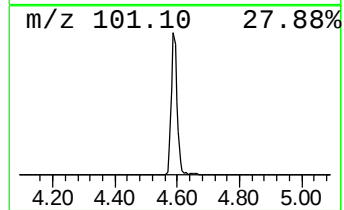
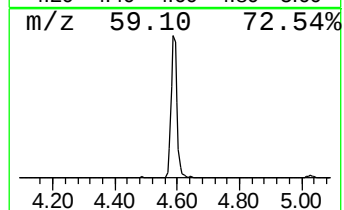
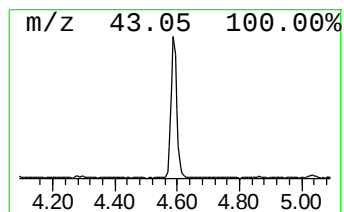
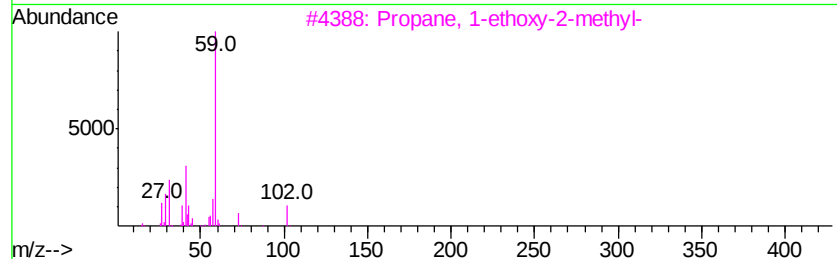
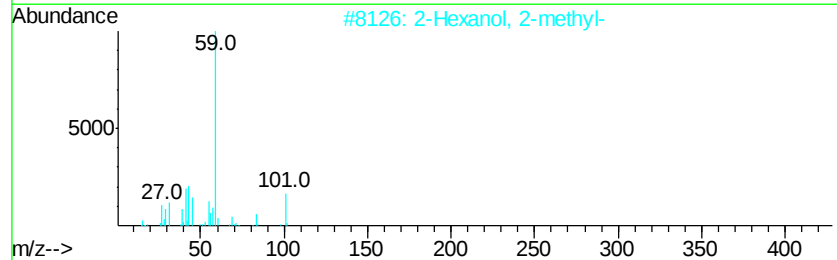
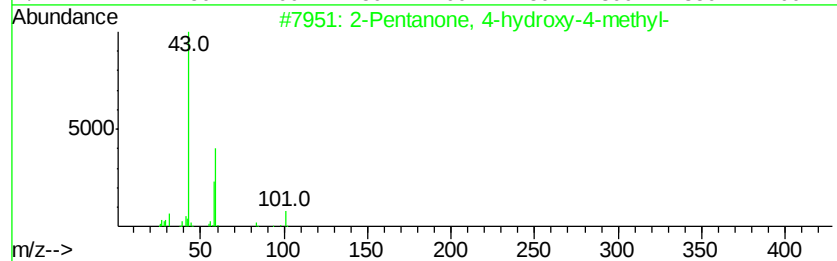
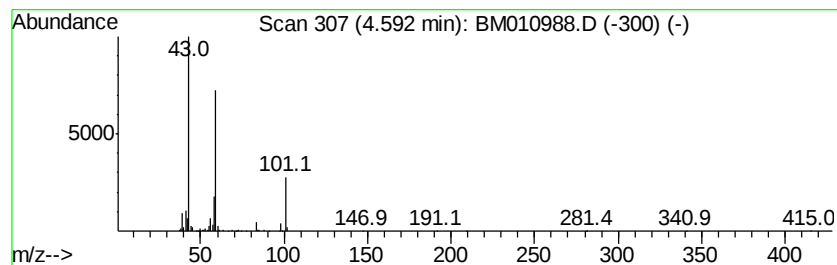
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	7.71 ng	775072	1,4-Dichlorobenzene-d4	7.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	53
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	27
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
5			1,2-Butanediol, (+/-)-	90	C4H10O2	026171-83-5	23



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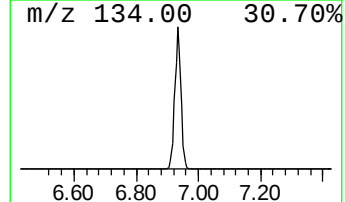
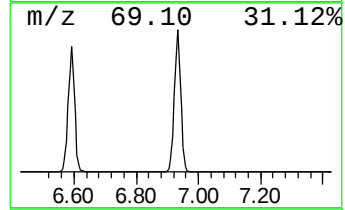
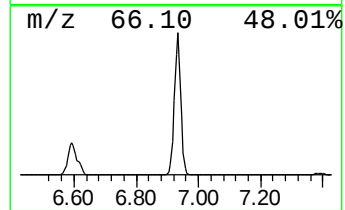
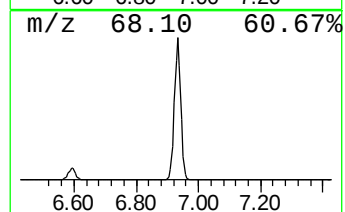
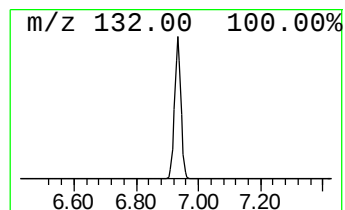
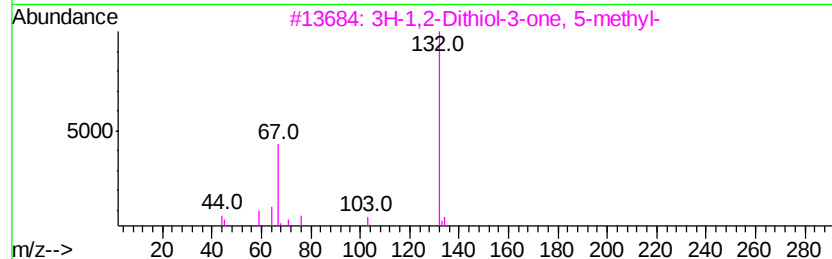
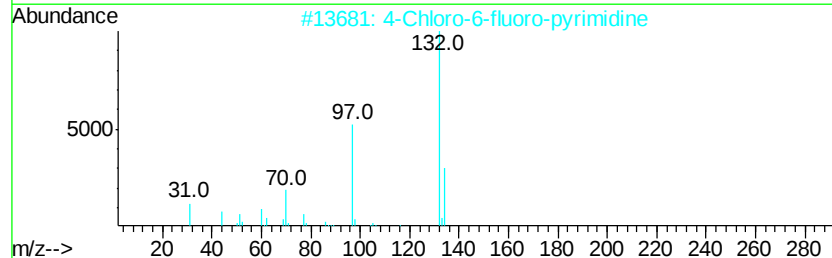
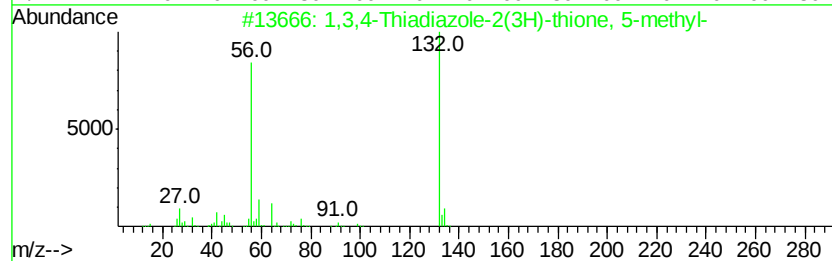
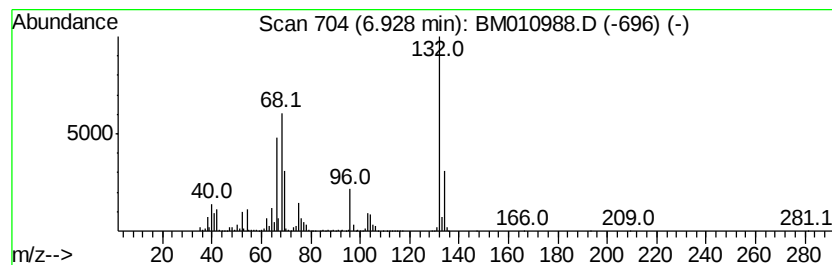
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Peak Number 2 unknown6.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.93	94.49 ng	9501630	1,4-Dichlorobenzene-d4	7.39

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
3		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	10
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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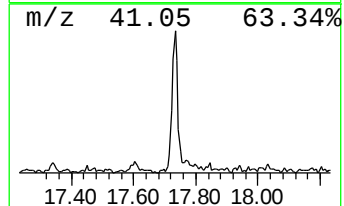
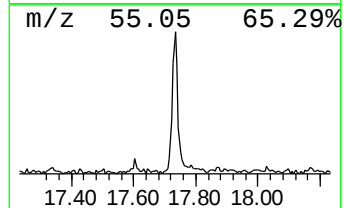
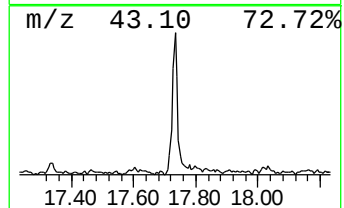
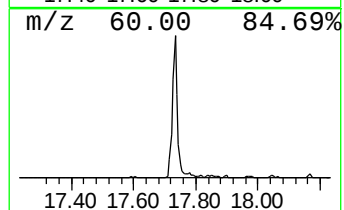
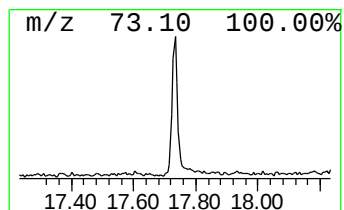
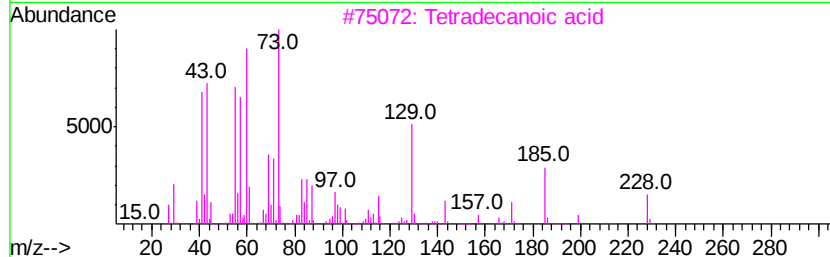
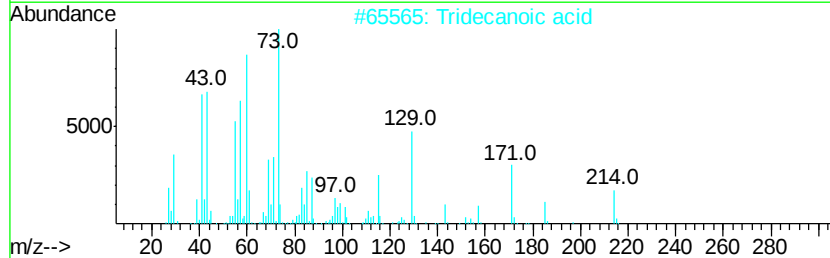
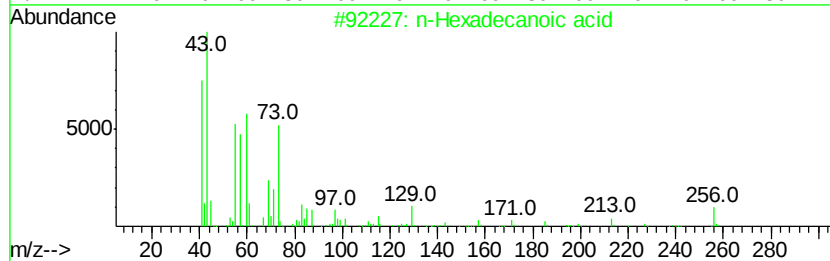
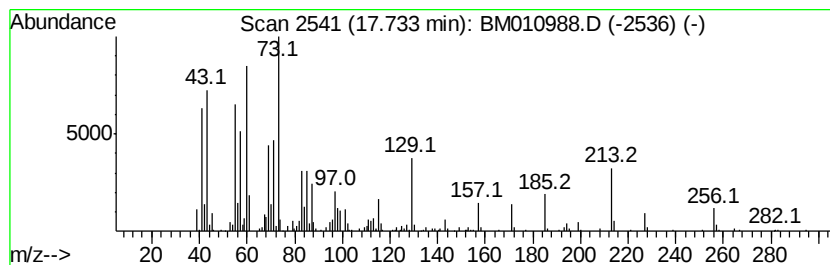
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.73	3.94 ng	868227	Phenanthrene-d10		16.80
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4	Dodecanoic acid	200	C12H24O2	000143-07-7	58
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	47



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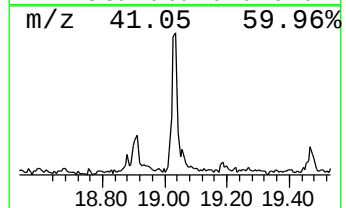
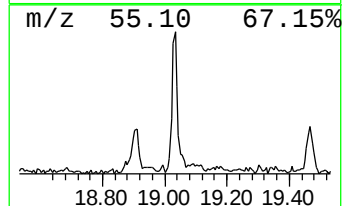
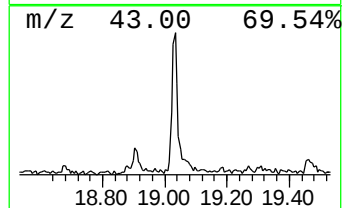
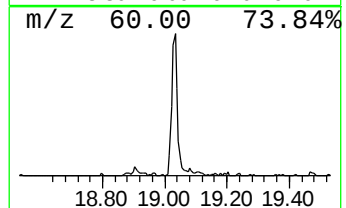
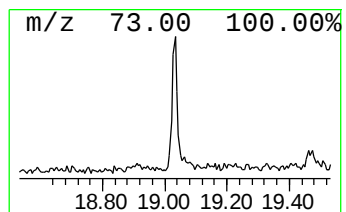
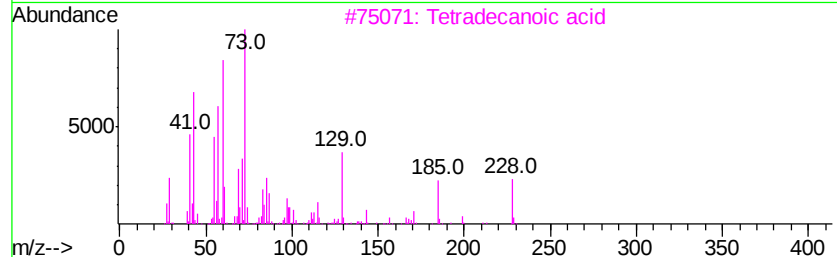
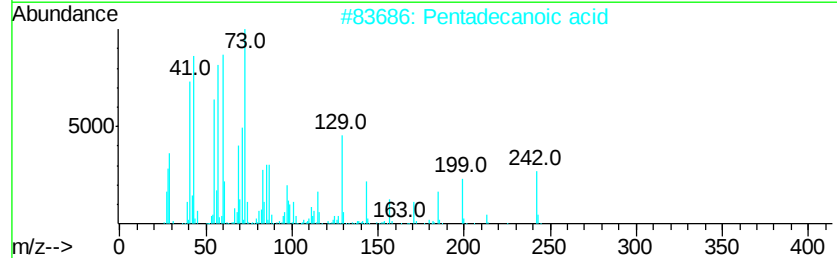
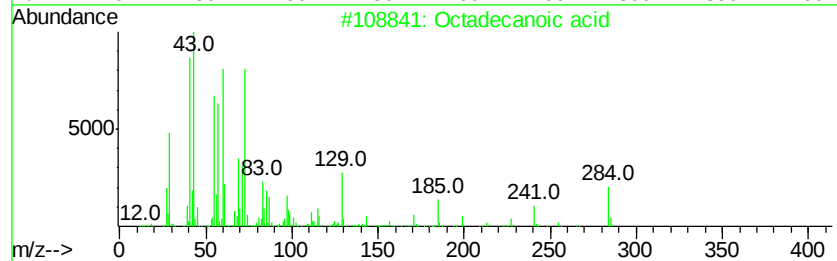
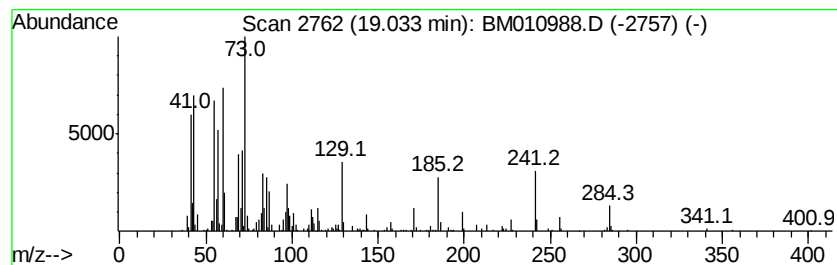
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.03	3.34 ng	691438	Chrysene-d12		21.02
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	95
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4	Octadecanoic acid, 2-(2-hydroxyve...	372	C22H44O4	000106-11-6	72
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.59	7.7	ng	775072	1	7.39	2011160	20.0
unknown6.93	6.93	94.5	ng	9501630	1	7.39	2011160	20.0
n-Hexadecanoic acid	17.73	3.9	ng	868227	4	16.80	4408880	20.0
Octadecanoic acid	19.03	3.3	ng	691438	5	21.02	4141080	20.0