

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052217\
 Data File : BM010116.D
 Acq On : 22 May 2017 23:24
 Operator : SJ/MA
 Sample : I3221-06
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 EX-04

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	4.652	262	266	271	rVB3	80637	118006	1.27%	0.242%
2	5.081	334	339	348	rBV	476264	673115	7.23%	1.382%
3	5.540	411	417	432	rBV	2300954	3407646	36.61%	6.995%
4	7.151	682	691	706	rBV	2146619	3419722	36.74%	7.020%
5	7.504	744	751	763	rBV	2274720	3592044	38.59%	7.373%
6	7.963	822	829	839	rVB	562512	918083	9.86%	1.885%
7	8.281	876	883	892	rVB	1782974	2916570	31.33%	5.987%
8	9.151	1023	1031	1039	rBV	1204207	2021697	21.72%	4.150%
9	10.769	1298	1306	1315	rBV	637256	1096237	11.78%	2.250%
10	13.216	1712	1722	1735	rBV	3498178	5073406	54.50%	10.414%
11	14.057	1858	1865	1872	rBV	452773	658912	7.08%	1.353%
12	14.592	1949	1956	1964	rBV2	990547	1515962	16.29%	3.112%
13	16.080	2203	2209	2220	rBV	2876038	4073142	43.76%	8.361%
14	17.339	2417	2423	2432	rBV	1421878	2024197	21.75%	4.155%
15	18.186	2562	2567	2575	rBV	317266	470218	5.05%	0.965%
16	19.051	2710	2714	2718	rBV5	63490	129992	1.40%	0.267%
17	19.457	2779	2783	2790	rBV5	117622	215260	2.31%	0.442%
18	19.939	2859	2865	2876	rBV	7806643	9308710	100.00%	19.108%
19	21.498	3125	3130	3135	rBV	2376543	3127946	33.60%	6.421%
20	22.650	3323	3326	3331	rVB	329886	428472	4.60%	0.880%
21	23.862	3526	3532	3544	rVB2	1728886	3527695	37.90%	7.241%

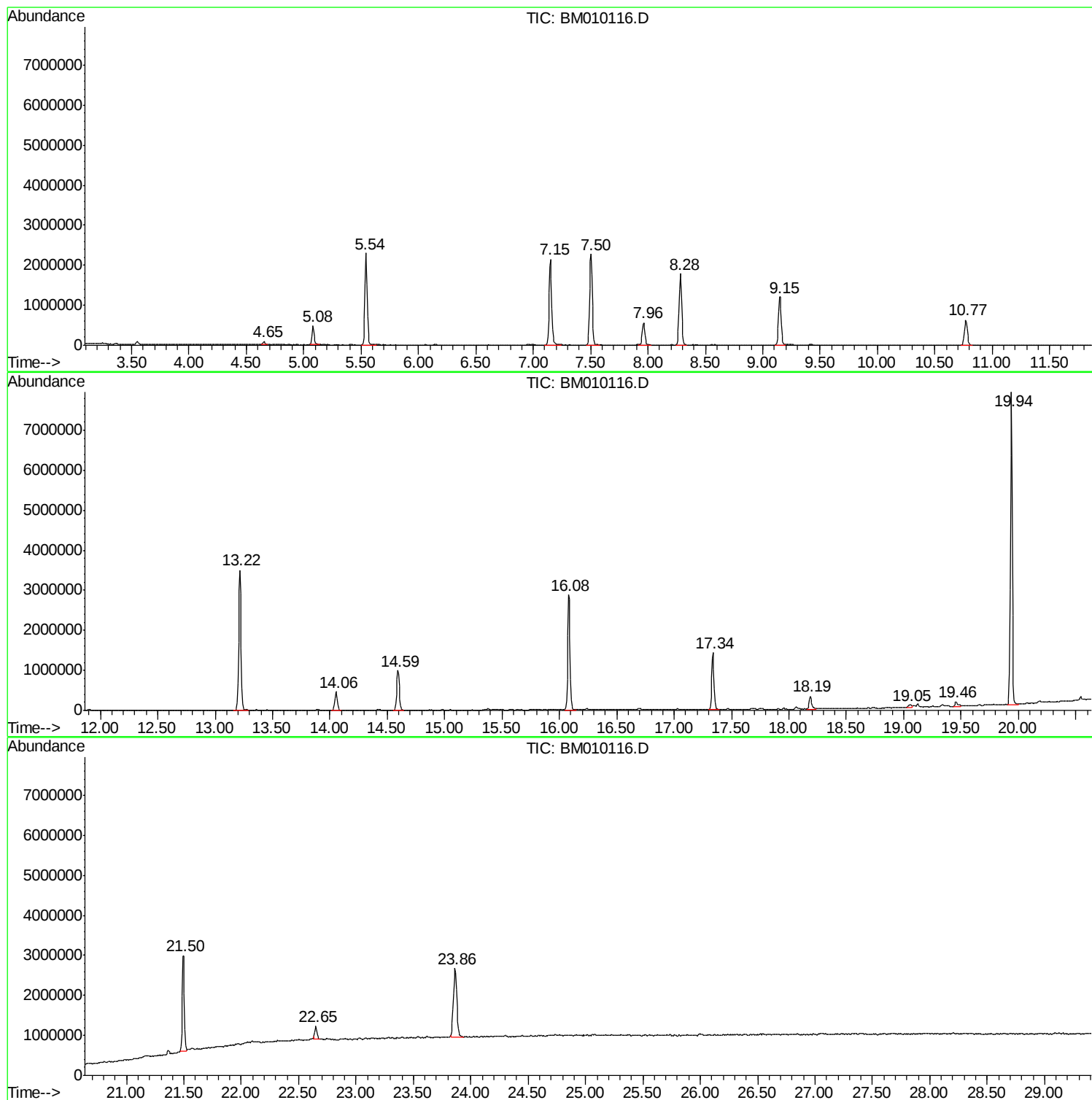
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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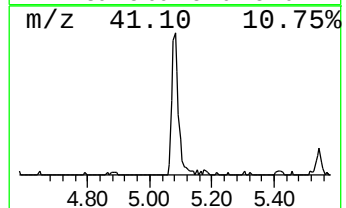
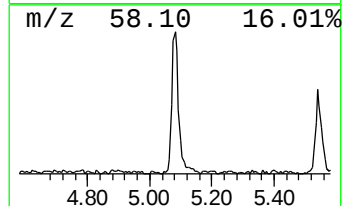
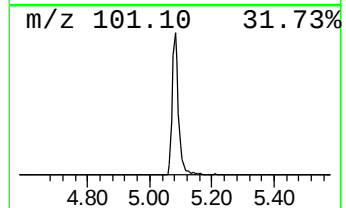
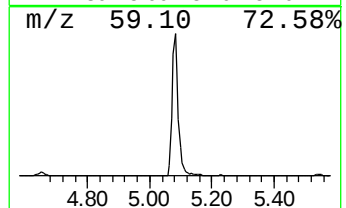
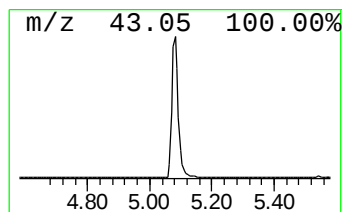
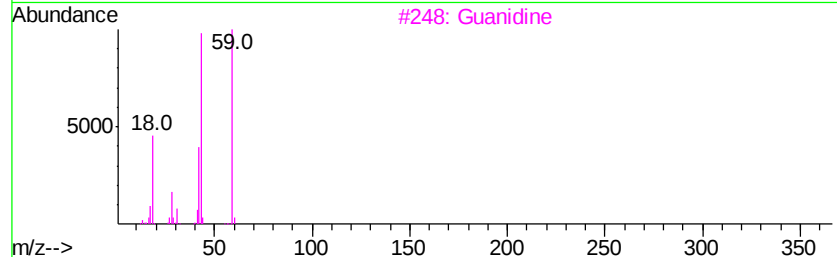
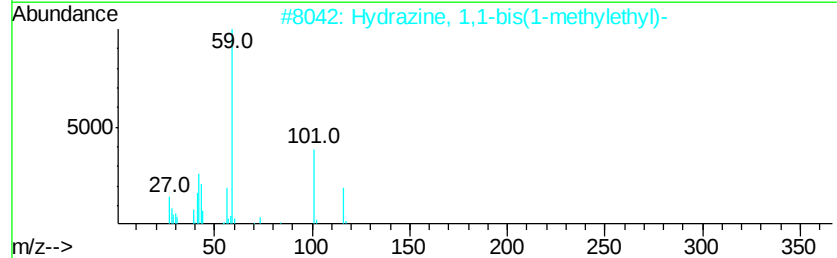
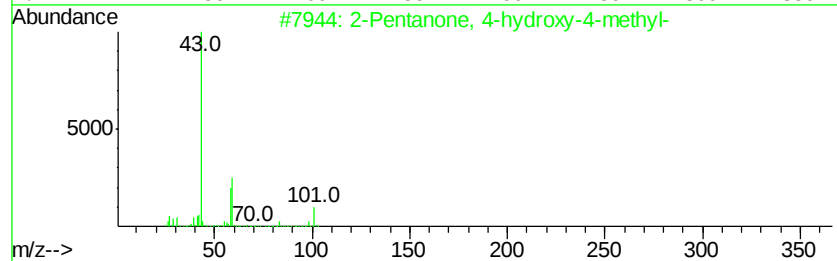
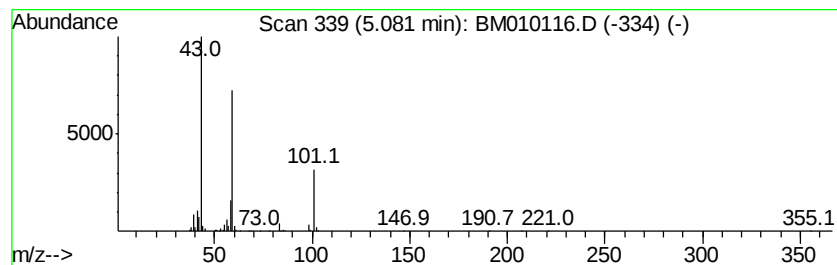
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.08	14.66 ng	673115	1,4-Dichlorobenzene-d4	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	47
3		Guanidine	59	CH5N3	000113-00-8	43
4		Dimethadione	129	C5H7NO3	000695-53-4	33
5		Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	23



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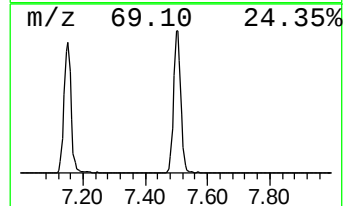
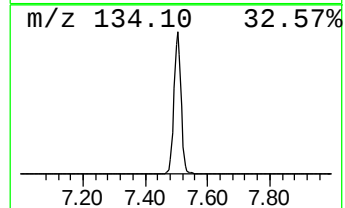
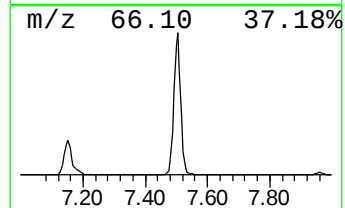
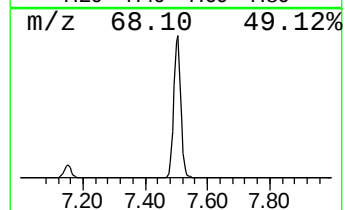
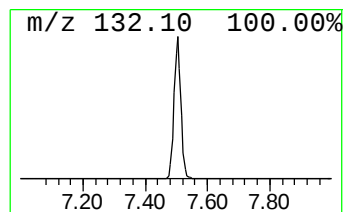
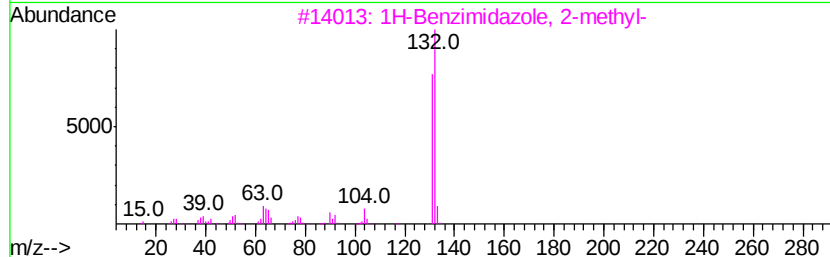
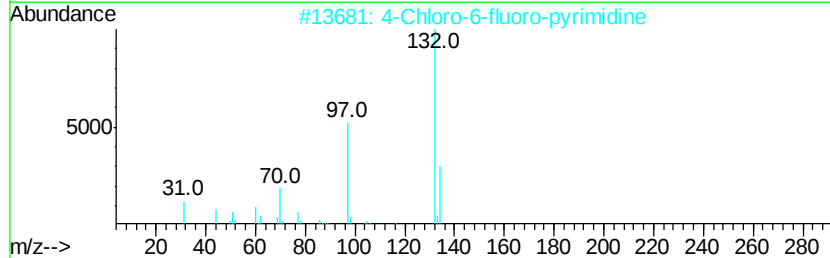
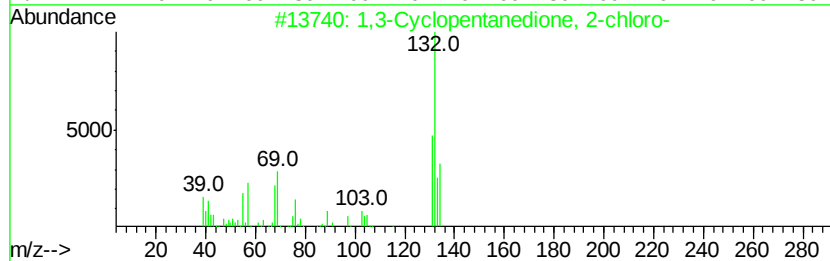
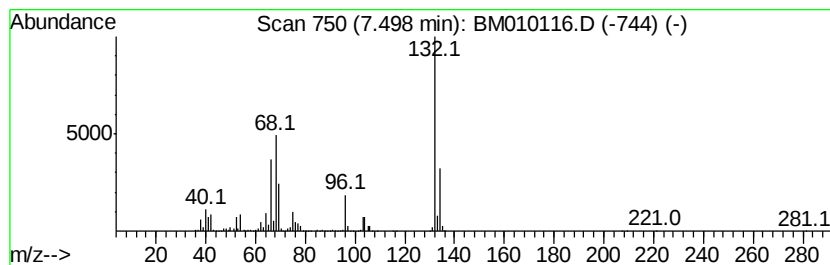
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Peak Number 3 unknown7.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	78.25 ng	3592040	1,4-Dichlorobenzene-d4	7.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	38
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16



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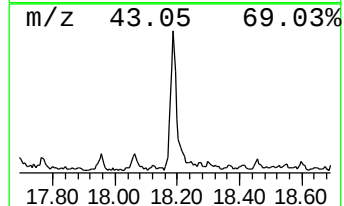
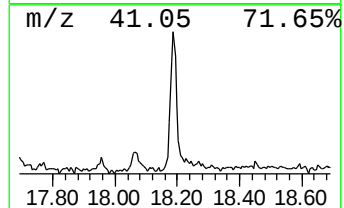
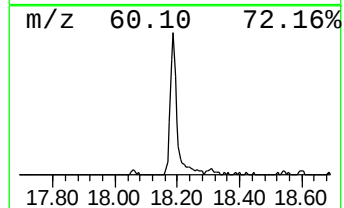
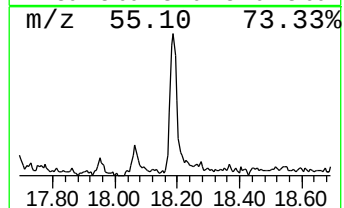
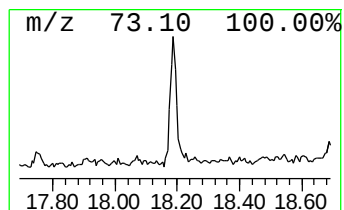
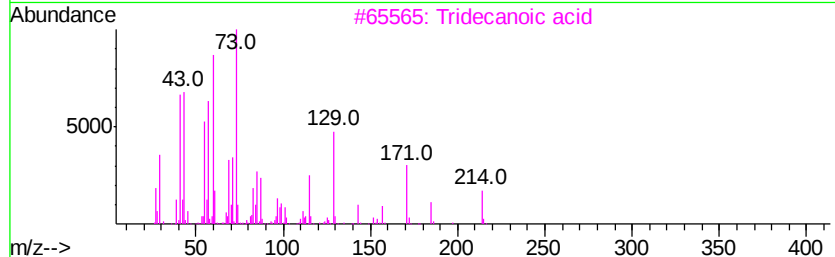
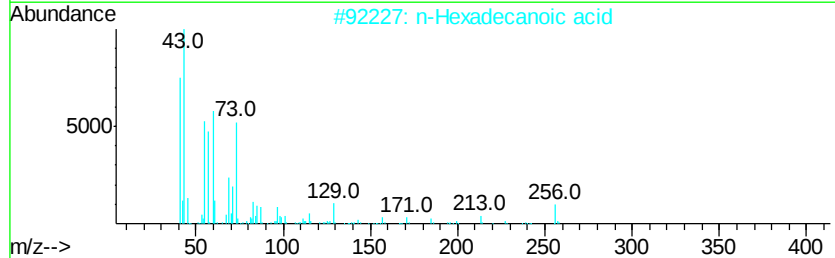
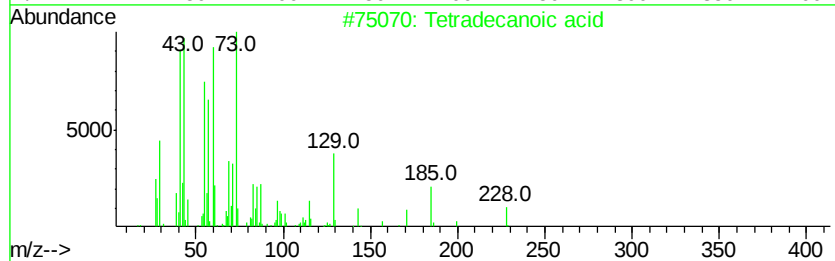
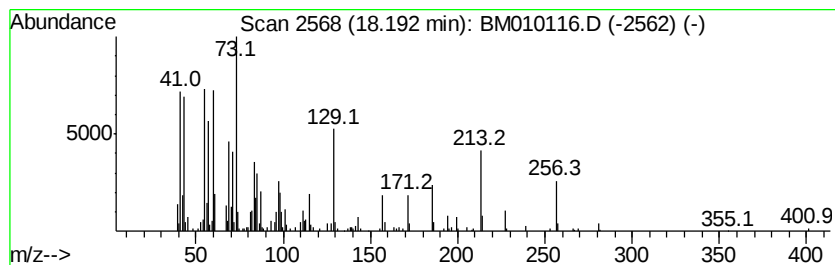
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Peak Number 5 Tetradecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.19	4.65 ng	470218	Phenanthrene-d10	17.34

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tetradecanoic acid	228	C14H28O2	000544-63-8	96
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	92
3		Tridecanoic acid	214	C13H26O2	000638-53-9	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	49
5		Undecanoic acid	186	C11H22O2	000112-37-8	49



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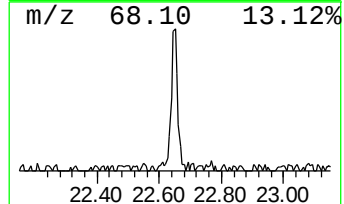
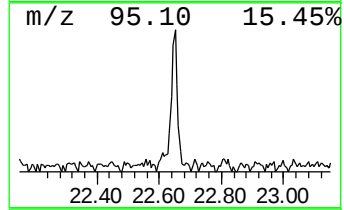
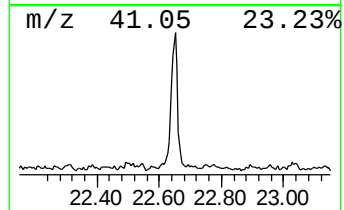
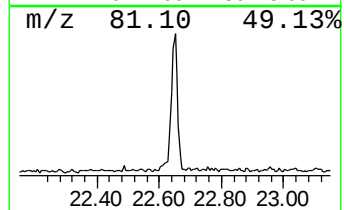
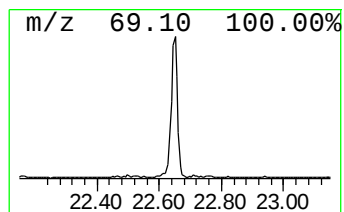
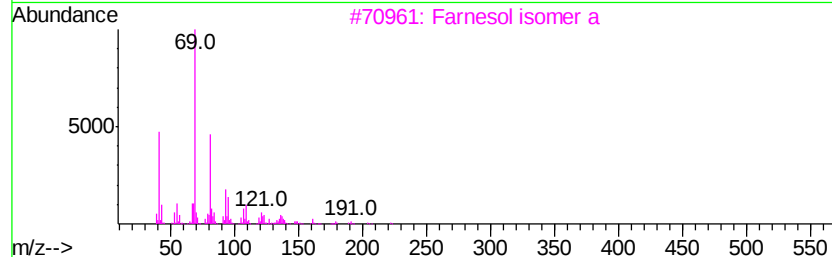
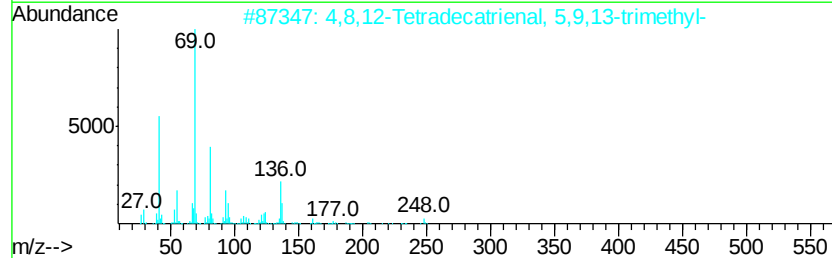
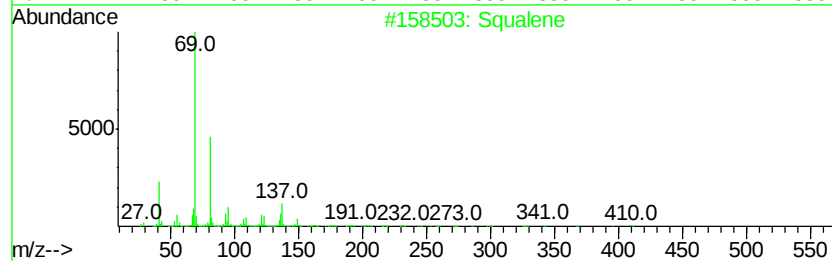
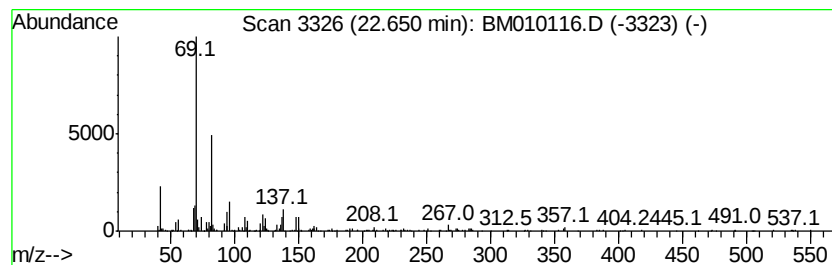
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.65	2.74 ng	428472	Chrysene-d12	21.50	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	007683-64-9	83
2	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	80
3	Farnesol isomer a	222	C15H26O	1000108-92-4	74
4	7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5	4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.08	14.7	ng	673115	1	7.96	918083	20.0
unknown7.50	7.50	78.3	ng	3592040	1	7.96	918083	20.0
Tetradecanoic acid	18.19	4.7	ng	470218	4	17.34	2024200	20.0
Squalene	22.65	2.7	ng	428472	5	21.50	3127950	20.0