

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM080618\
 Data File : BM016206.D
 Acq On : 07 Aug 2018 00:13
 Operator : SJ/JU
 Sample : J4330-06
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 073018-DBRI-E-U-S

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_M\METHODS\8270-BM072318.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	5.692	404	409	429	rBV	315102	510218	15.90%	3.605%
2	7.334	683	688	700	rBV	189119	329113	10.26%	2.326%
3	7.698	744	750	763	rBV	640169	1053358	32.84%	7.443%
4	8.169	824	830	842	rBB	186444	304650	9.50%	2.153%
5	8.492	878	885	899	rVB	893902	1449903	45.20%	10.245%
6	9.357	1025	1032	1045	rBV	716724	1178932	36.75%	8.331%
7	10.986	1303	1309	1323	rBV	209534	356761	11.12%	2.521%
8	13.421	1717	1723	1732	rVB	1608383	2254419	70.28%	15.930%
9	14.798	1952	1957	1966	rBB2	269086	408739	12.74%	2.888%
10	16.068	2169	2173	2179	rBV	54339	61418	1.91%	0.434%
11	16.286	2204	2210	2219	rBV	878632	1158881	36.13%	8.189%
12	17.533	2417	2422	2430	rBV2	334037	473772	14.77%	3.348%
13	18.380	2561	2566	2574	rBV2	56317	77542	2.42%	0.548%
14	19.639	2776	2780	2787	rBV4	27001	36365	1.13%	0.257%
15	20.109	2855	2860	2866	rBV	2687850	3207975	100.00%	22.669%
16	21.662	3119	3124	3130	rBV	462471	583875	18.20%	4.126%
17	22.821	3318	3321	3326	rVB	94962	127890	3.99%	0.904%
18	24.015	3517	3524	3531	rVB	292713	577859	18.01%	4.083%

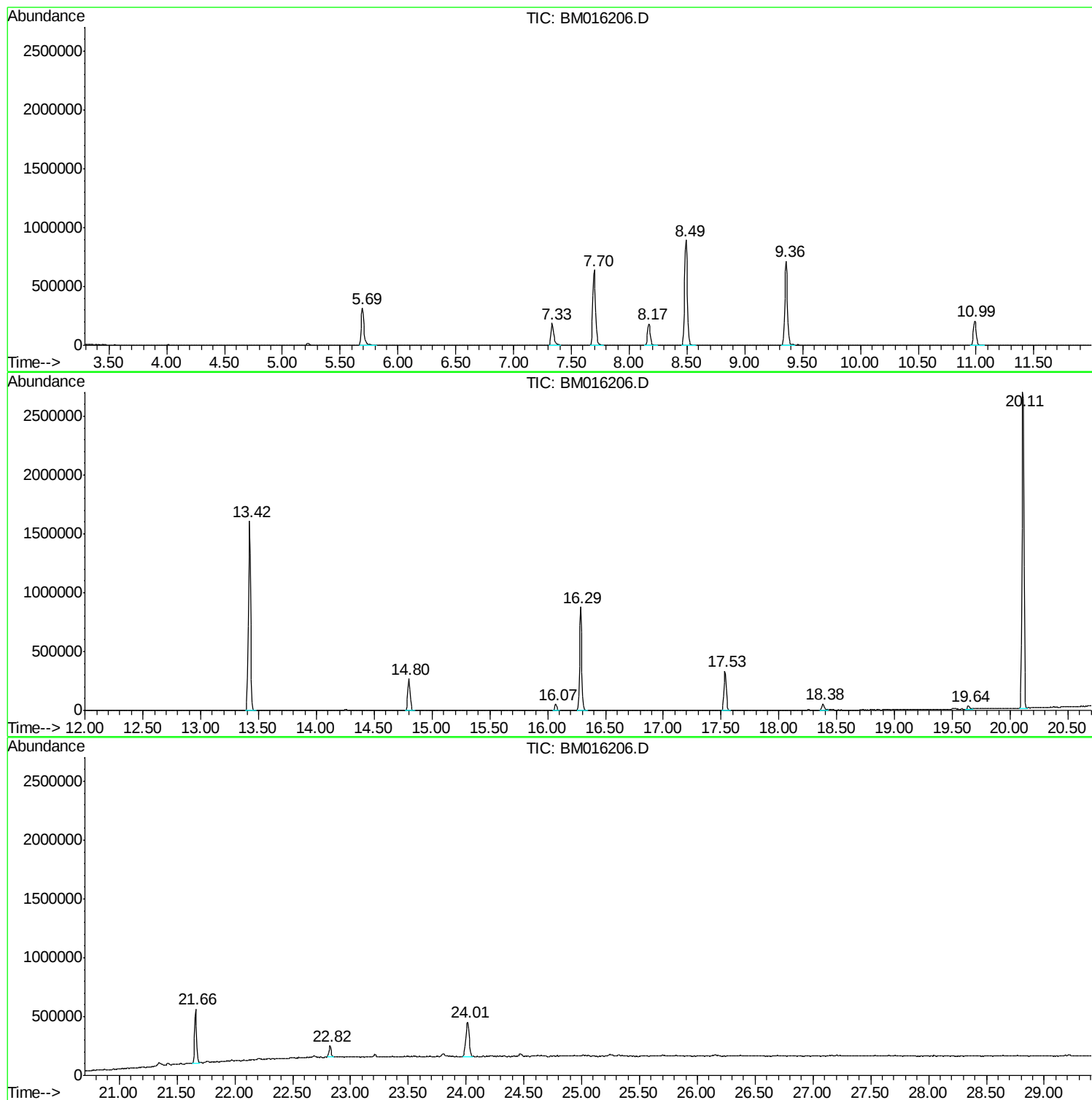
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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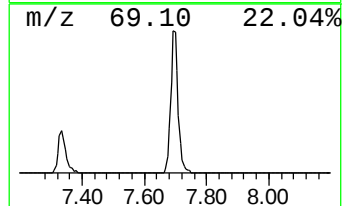
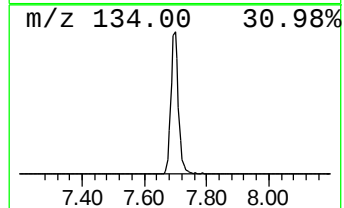
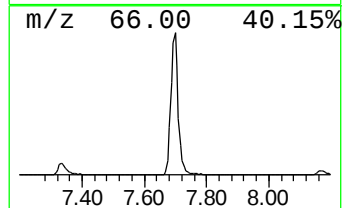
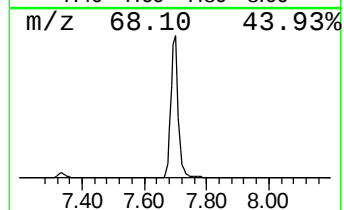
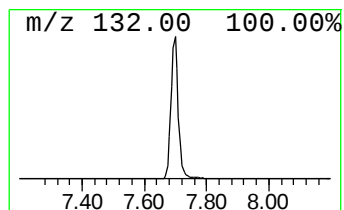
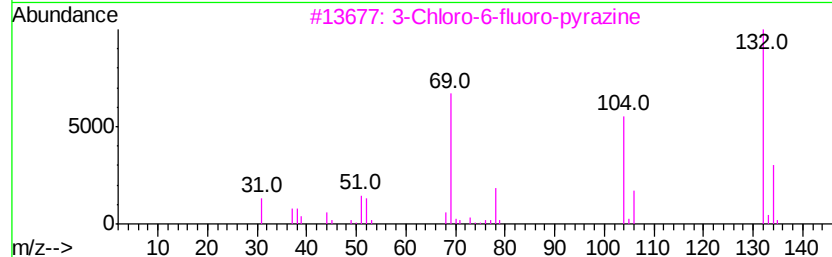
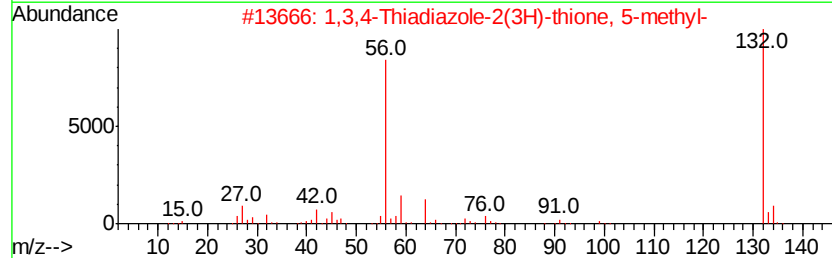
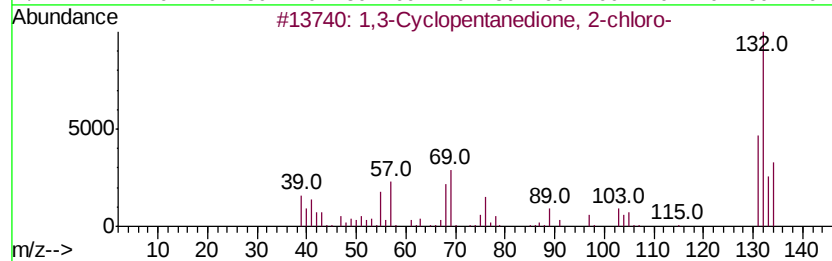
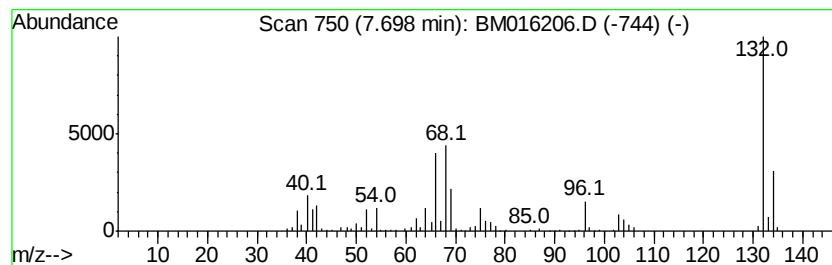
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM072318.M
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.70 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.70	69.15 ng	1053360	1,4-Dichlorobenzene-d4	8.17

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	27
2			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
5			3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	14



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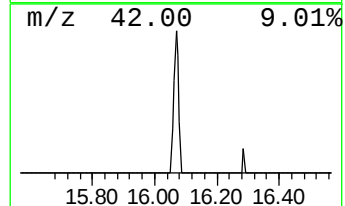
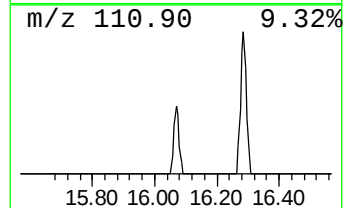
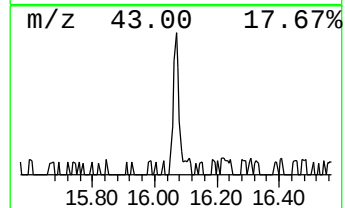
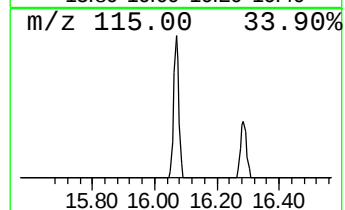
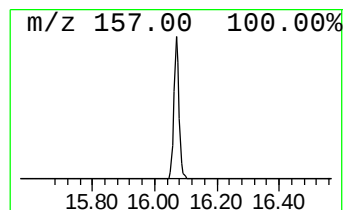
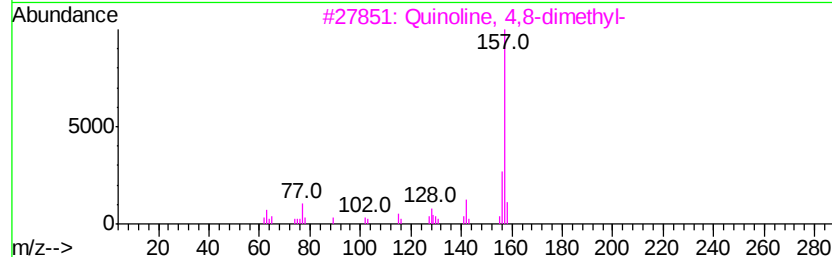
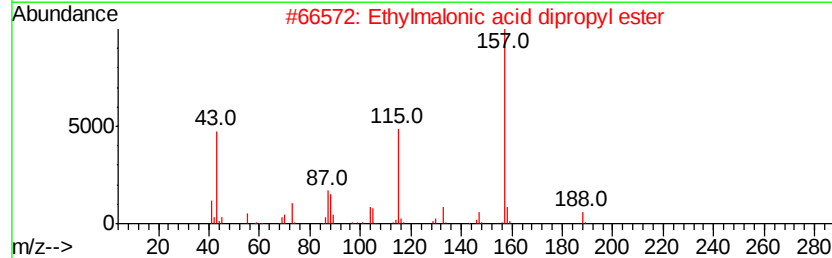
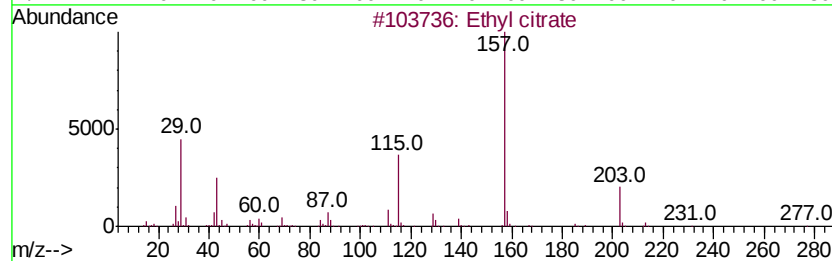
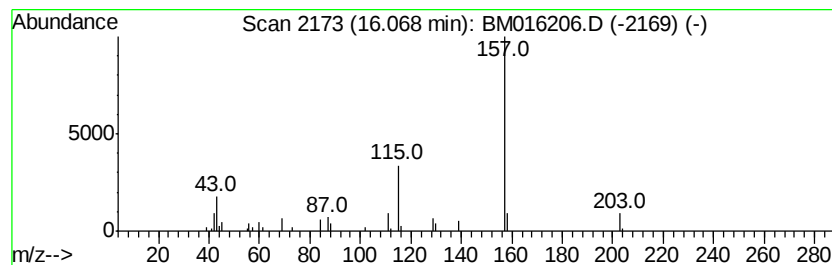
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Peak Number 3 Ethyl citrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.07	3.01 ng	61418	Acenaphthene-d10	14.80

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethyl citrate	276	C12H20O7	000077-93-0	90
2		Ethylmalonic acid dipropyl ester	216	C11H20O4	001113-91-3	56
3		Quinoline, 4,8-dimethyl-	157	C11H11N	013362-80-6	40
4		1-Amino-2-methylnaphthalene	157	C11H11N	002246-44-8	33
5		2-Fluoro-6-nitrophenol	157	C6H4FN03	001526-17-6	33



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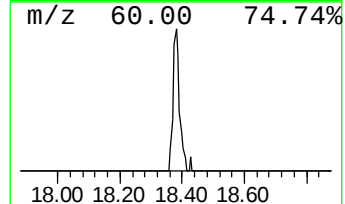
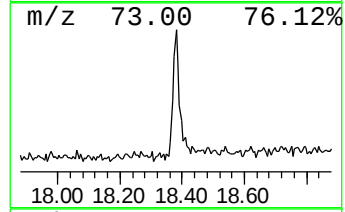
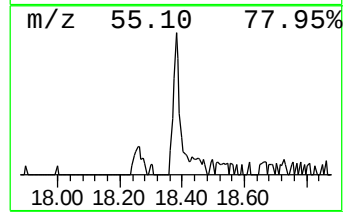
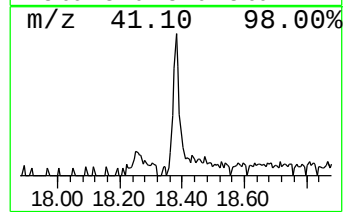
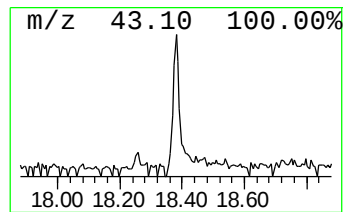
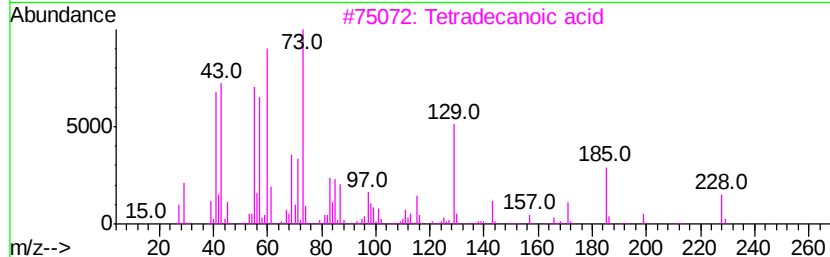
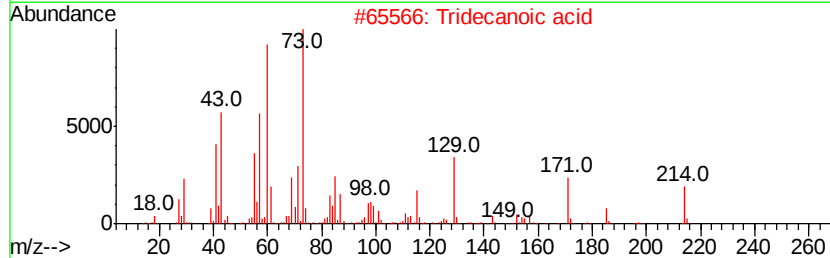
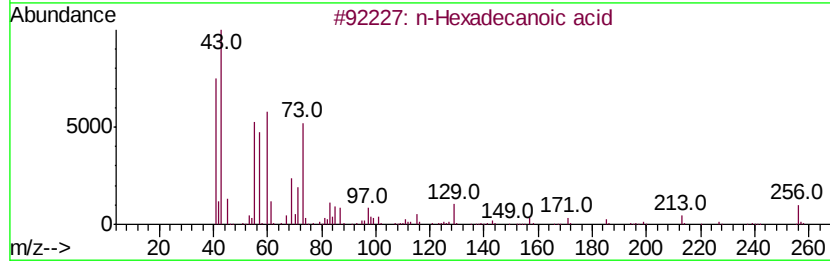
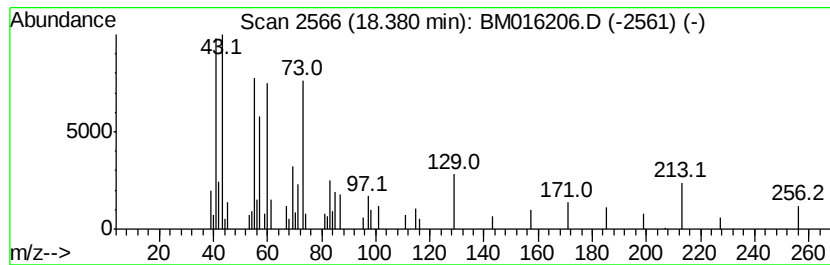
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.38	3.27 ng	77542	Phenanthrene-d10	17.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Tridecanoic acid	214	C13H26O2	000638-53-9	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Dodecanoic acid	200	C12H24O2	000143-07-7	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



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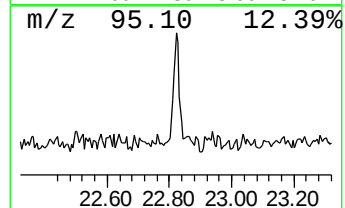
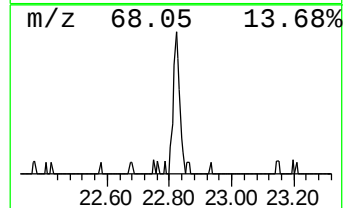
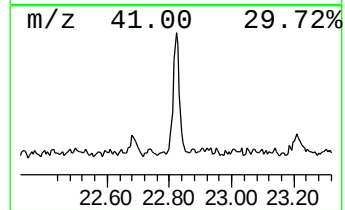
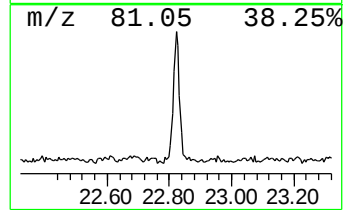
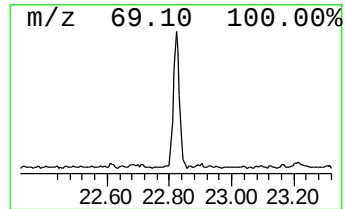
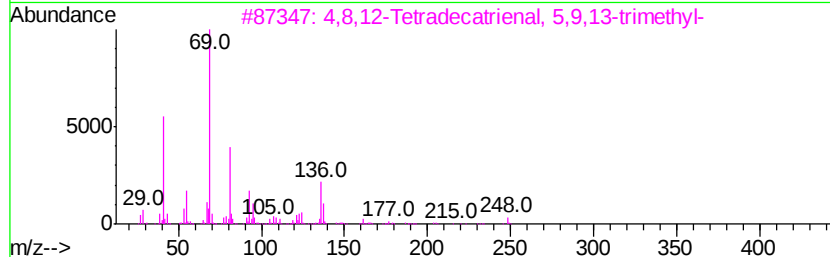
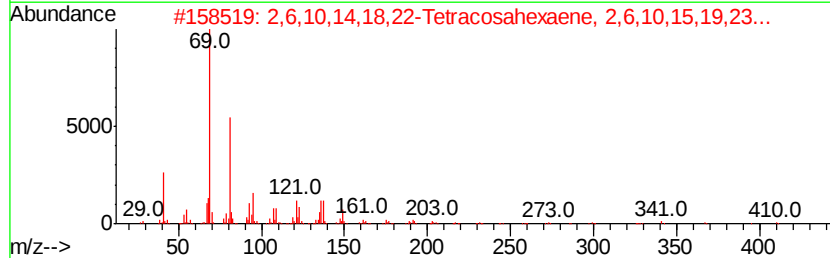
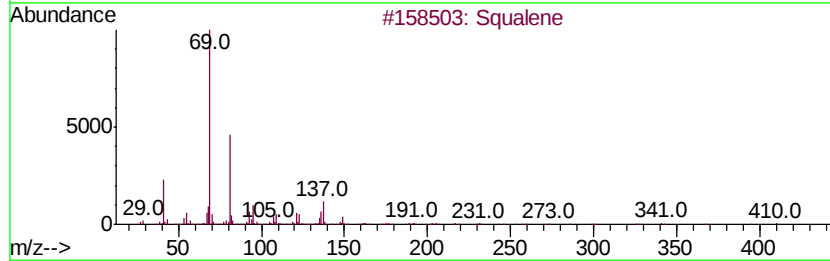
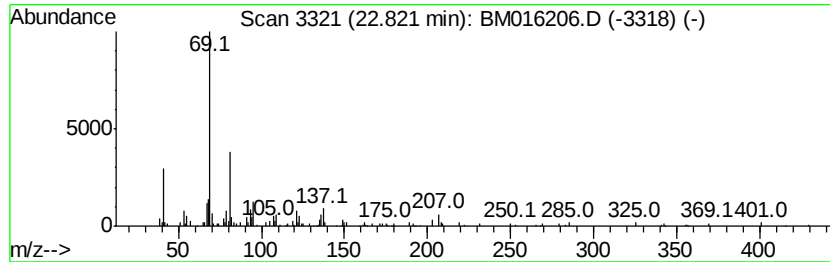
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Peak Number 5 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.82	4.38 ng	127890	Chrysene-d12	21.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	83
2		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	72
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
5		1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Ethyl citrate	16.07	3.0	ng	61418	3	14.80	408739	20.0
n-Hexadecanoic acid	18.38	3.3	ng	77542	4	17.53	473772	20.0
Squalene	22.82	4.4	ng	127890	5	21.66	583875	20.0