

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG072115\
 Data File : BG018043.D
 Acq On : 22 Jul 2015 4:56
 Operator : TP/UM
 Sample : G3007-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S-2(8.0-8.5)

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_G\METHODS\8270-BG071715.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	2.806	16	20	25	rBV	116637	135540	3.19%	0.607%
2	4.692	336	341	347	rVB	86783	117480	2.76%	0.526%
3	5.156	413	420	432	rVB	936484	1335791	31.42%	5.979%
4	6.736	680	689	701	rBV	1049740	1618617	38.07%	7.245%
5	7.083	741	748	758	rVB	1090613	1717091	40.39%	7.686%
6	7.547	820	827	835	rVB	187989	296653	6.98%	1.328%
7	7.864	874	881	888	rBV	812121	1254387	29.50%	5.615%
8	8.705	1017	1024	1033	rVB	657792	1072956	25.24%	4.803%
9	10.326	1293	1300	1306	rBV	291322	483056	11.36%	2.162%
10	12.823	1718	1725	1733	rBV	1988047	2902114	68.26%	12.991%
11	13.675	1864	1870	1879	rBV	838811	1109416	26.09%	4.966%
12	14.210	1951	1961	1969	rBV2	490871	745925	17.54%	3.339%
13	15.708	2209	2216	2225	rBV	1690993	2334261	54.90%	10.449%
14	16.960	2423	2429	2435	rBV2	530615	793420	18.66%	3.552%
15	17.882	2581	2586	2593	rBV4	57477	95853	2.25%	0.429%
16	19.615	2874	2881	2895	rVB	3317147	4251543	100.00%	19.031%
17	21.161	3139	3144	3150	rBV	741826	980052	23.05%	4.387%
18	22.336	3339	3344	3349	rBV	90083	126789	2.98%	0.568%
19	23.364	3512	3519	3527	rVB2	506364	968916	22.79%	4.337%

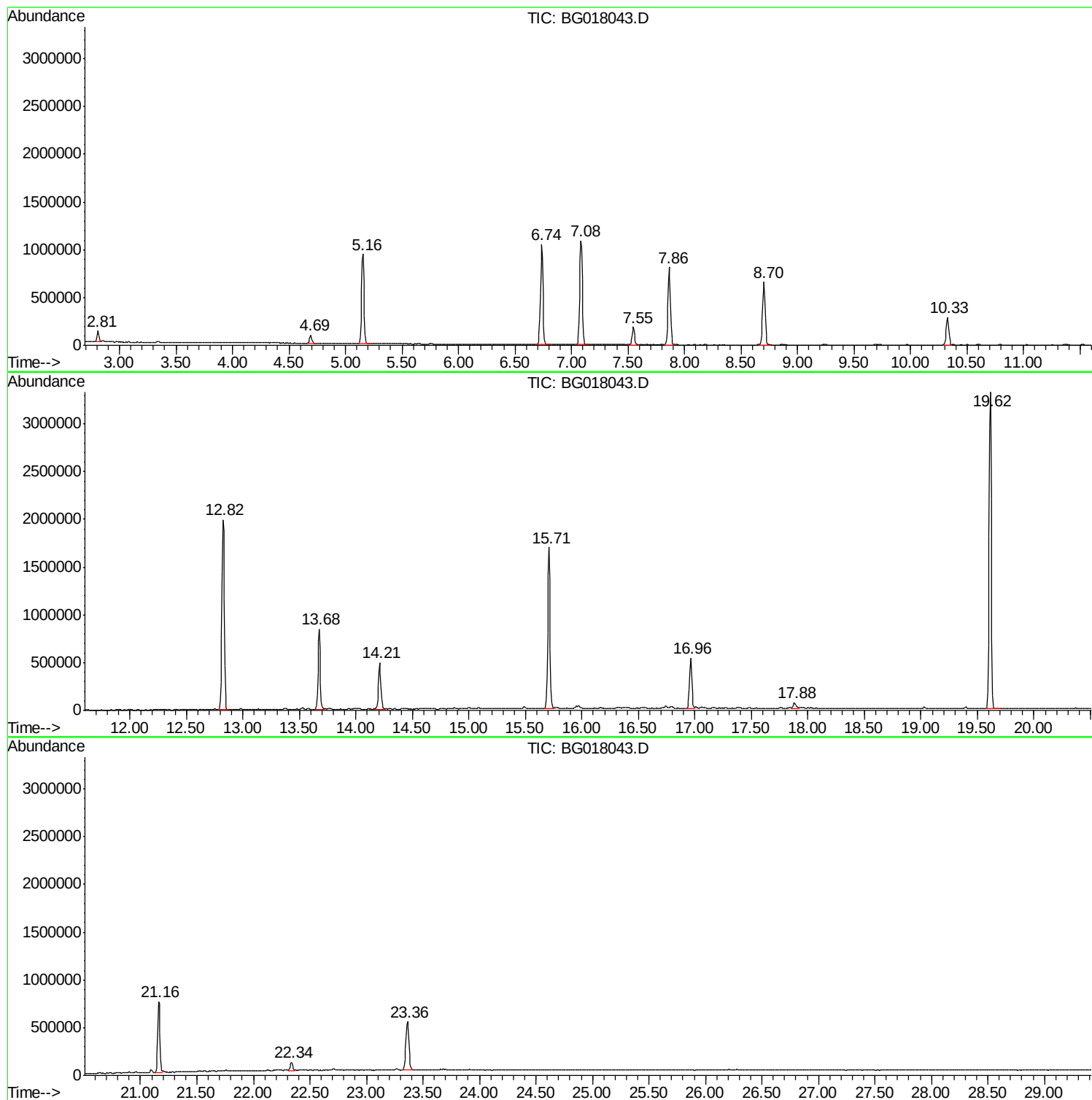
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S-2(8.0-8.5)

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG071715.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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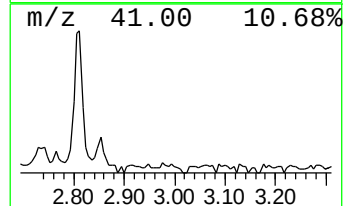
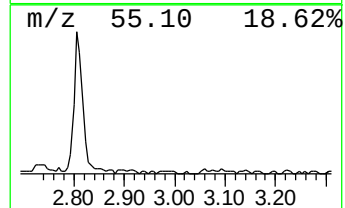
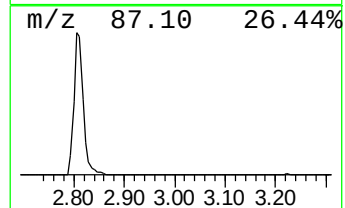
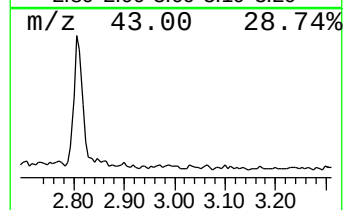
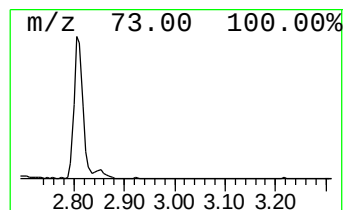
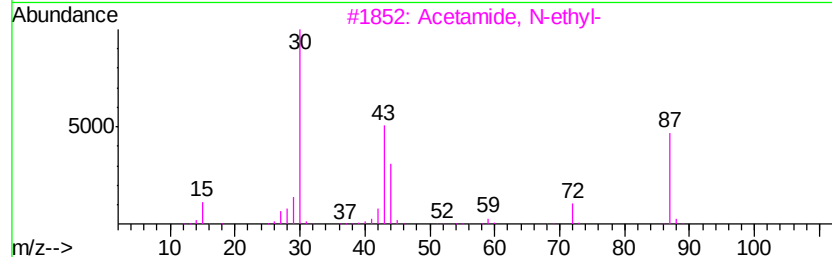
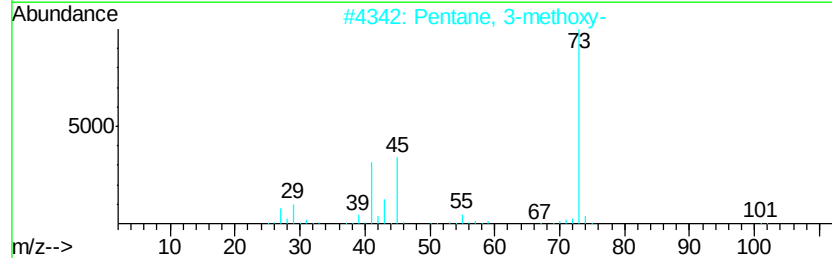
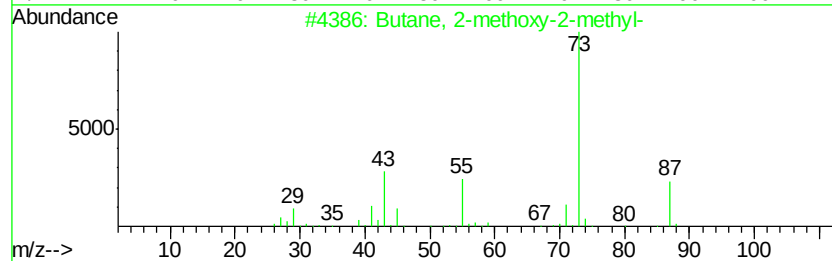
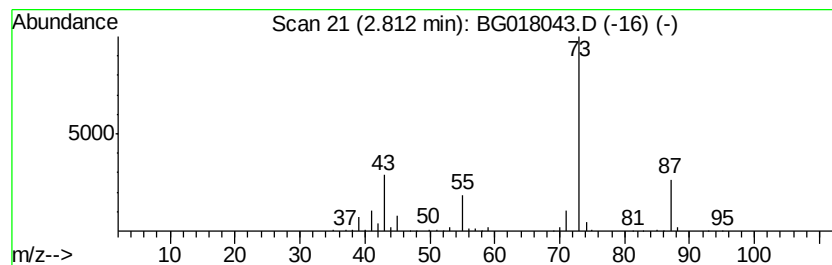
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.81	9.14 ng	135540	1,4-Dichlorobenzene-d4	7.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1-Propene-1-thiol	74	C3H6S	000925-89-3	5



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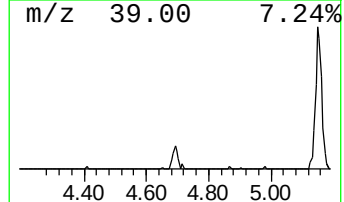
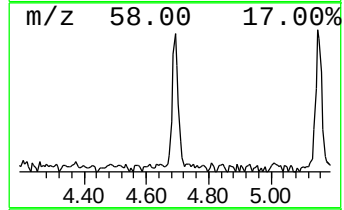
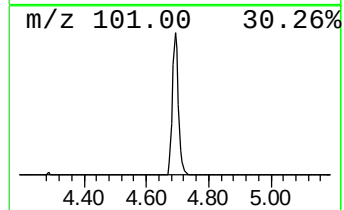
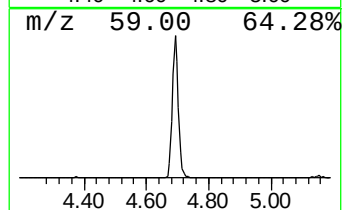
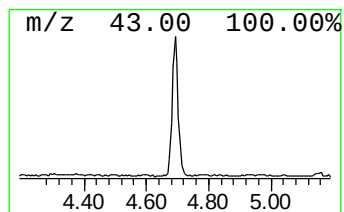
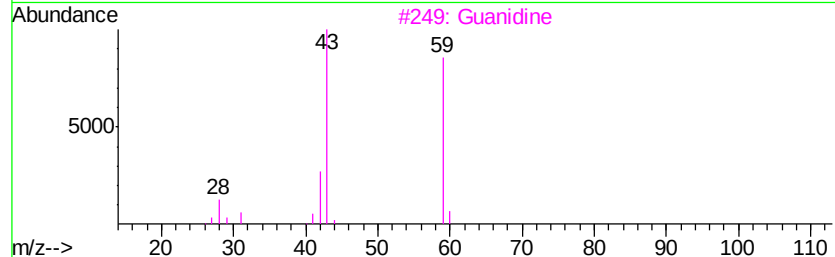
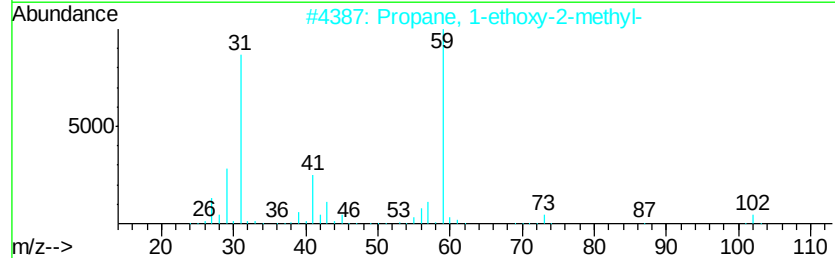
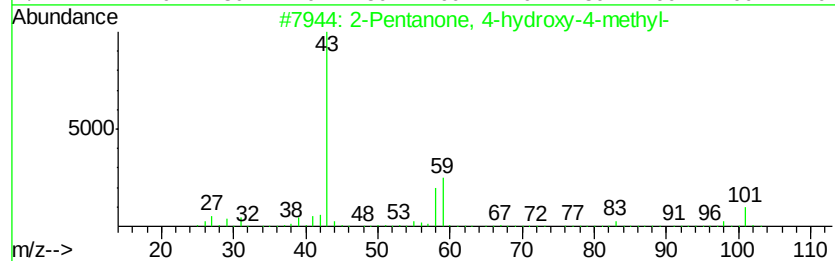
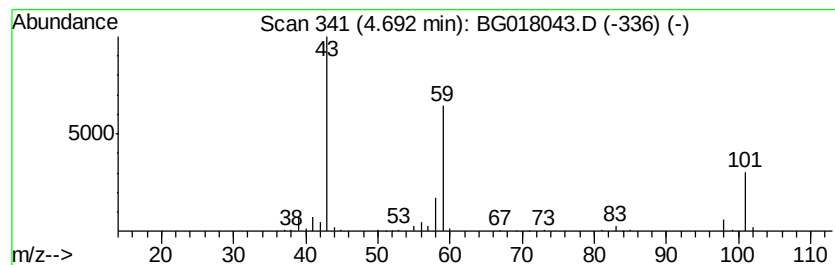
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.69	7.92 ng	117480	1,4-Dichlorobenzene-d4	7.55

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9
3			Guanidine	59	CH5N3	000113-00-8	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7N2O2	016504-58-8	9



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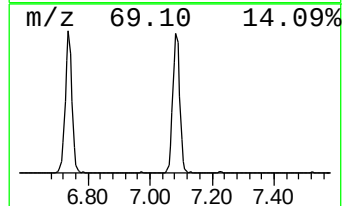
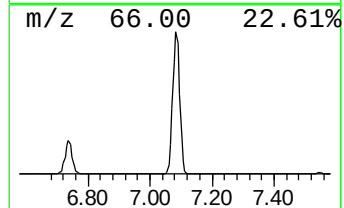
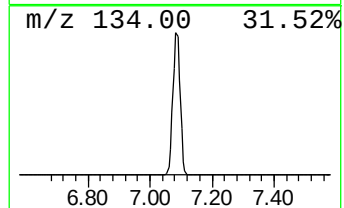
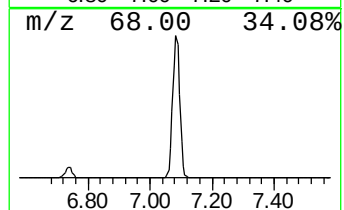
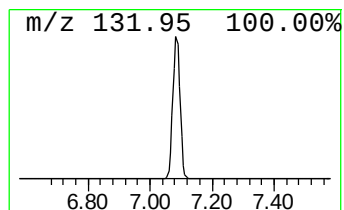
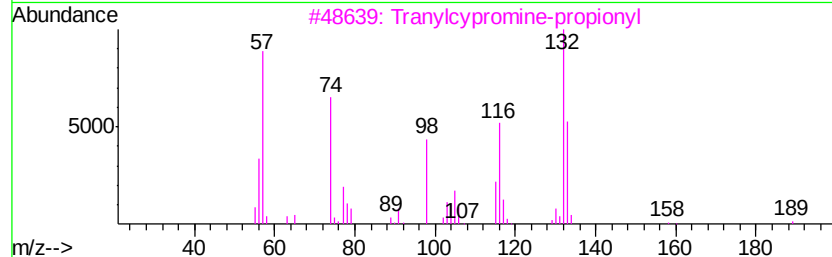
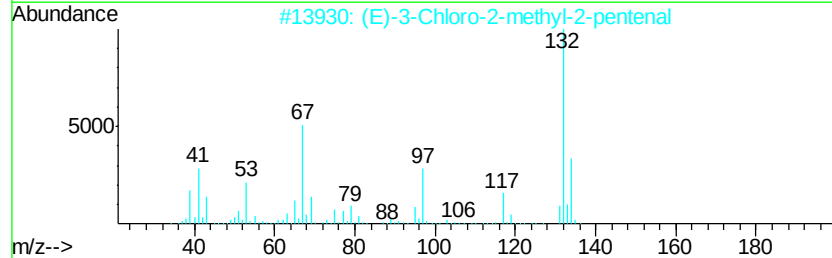
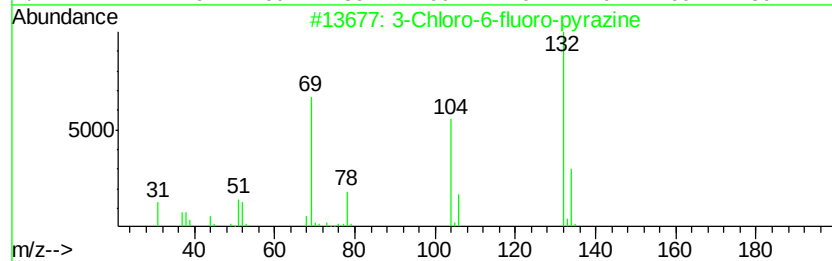
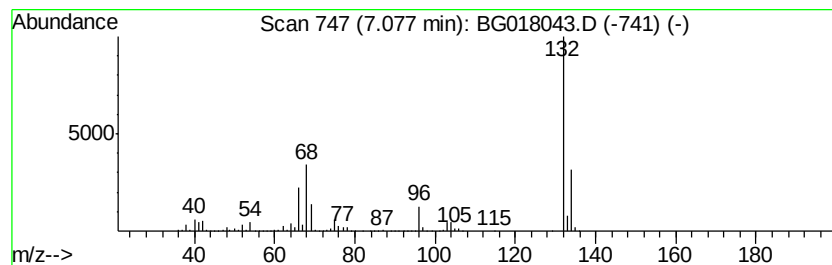
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Peak Number 3 unknown7.08 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.08	115.76 ng	1717090	1,4-Dichlorobenzene-d4	7.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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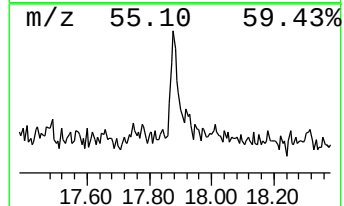
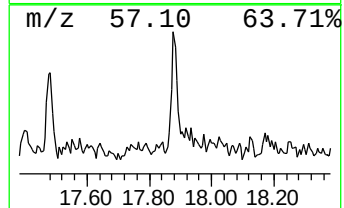
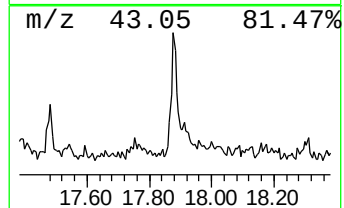
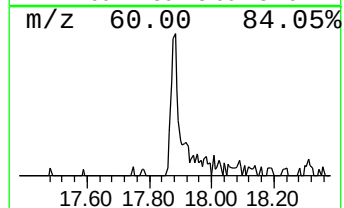
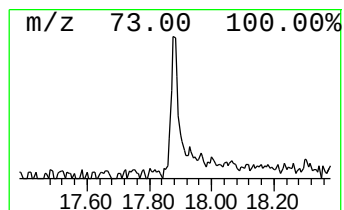
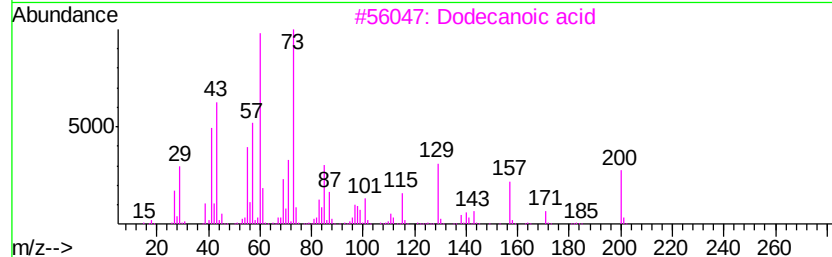
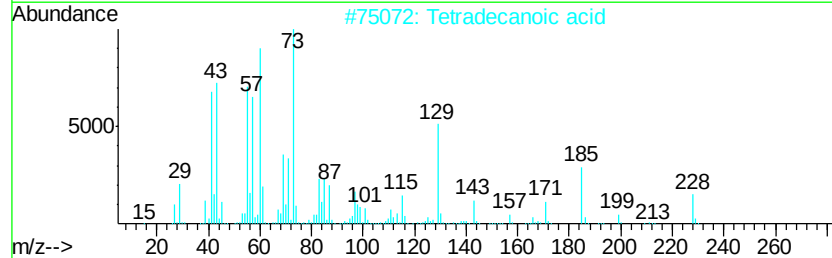
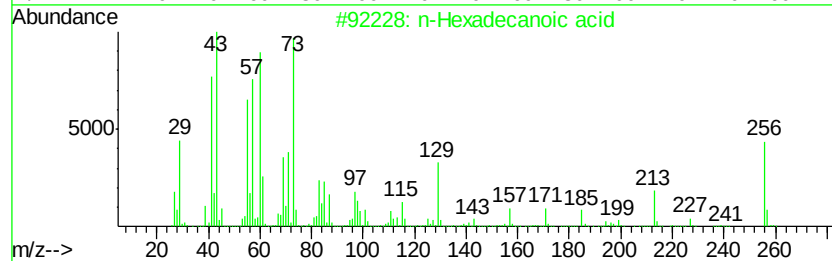
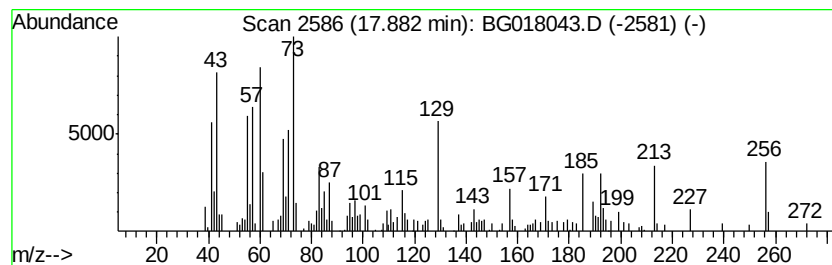
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.88	2.42 ng	95853	Phenanthrene-d10		16.96
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	89
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	58
3	Dodecanoic acid	200	C12H24O2	000143-07-7	47
4	n-Decanoic acid	172	C10H20O2	000334-48-5	44
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	43



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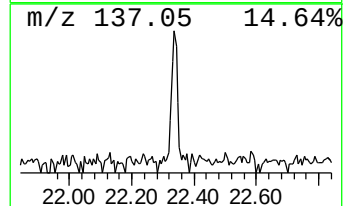
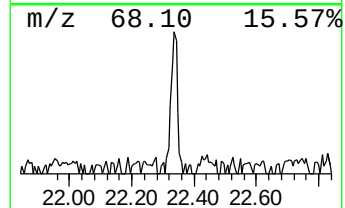
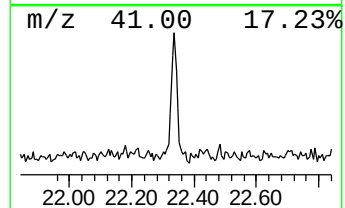
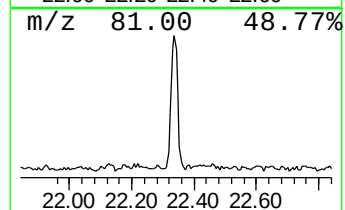
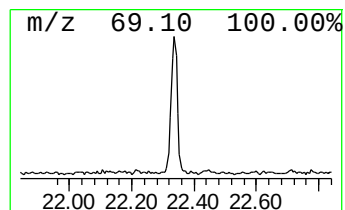
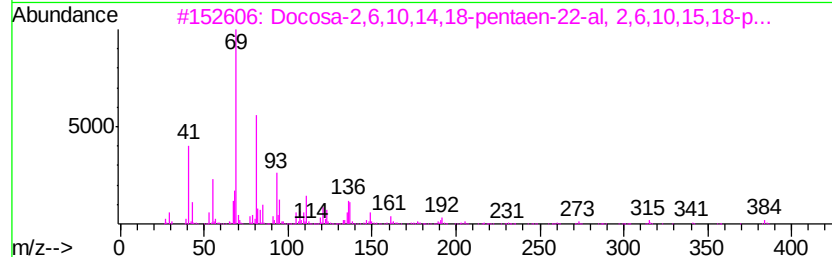
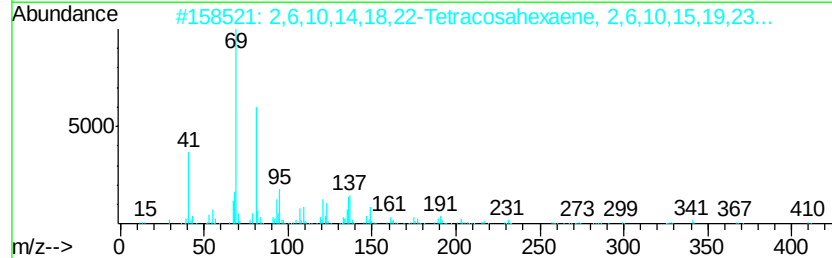
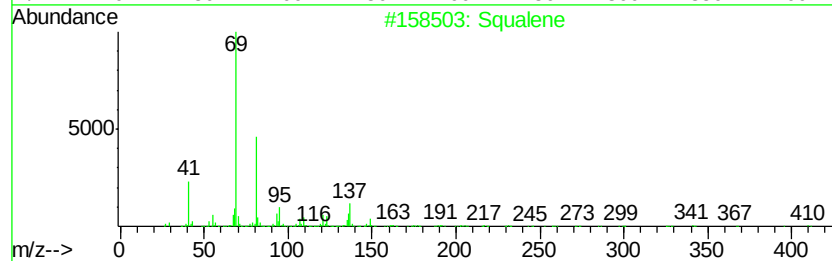
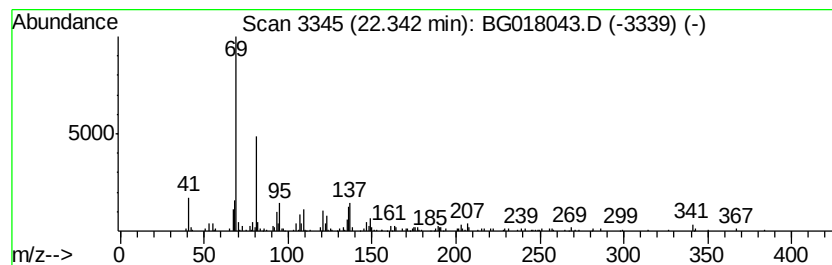
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.34	2.62 ng	126789	Perylene-d12	23.36
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Squalene	410 C30H50	007683-64-9	96
2	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	96
3	Docosa-2,6,10,14,18-pentaen-22-a...	384 C27H44O	1000163-04-7	87
4	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	78
5	2,6,10,14-Hexadecatetraen-1-ol, ...	332 C22H36O2	061691-98-3	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.81	9.1	ng	135540	1	7.55	296653	20.0
2-Pentanone, 4-hy...	4.69	7.9	ng	117480	1	7.55	296653	20.0
unknown7.08	7.08	115.8	ng	1717090	1	7.55	296653	20.0
n-Hexadecanoic acid	17.88	2.4	ng	95853	4	16.96	793420	20.0
Squalene	22.34	2.6	ng	126789	6	23.36	968916	20.0