

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
 Data File : BG023424.D
 Acq On : 3 Aug 2016 13:58
 Operator : UM/SJ
 Sample : H4287-06
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-59-19.0-20.0

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-BG080116.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	2.999	22	27	41	rVB	2075617	3030626	28.62%	5.080%
2	5.196	394	401	408	rBV	619631	942472	8.90%	1.580%
3	5.672	475	482	498	rBV	2205011	3547906	33.50%	5.947%
4	7.293	750	758	769	rBV	2424728	4313650	40.73%	7.230%
5	7.663	811	821	839	rBV	2291185	4019175	37.95%	6.736%
6	8.133	895	901	909	rBV	443710	761008	7.19%	1.276%
7	8.462	949	957	968	rBV	1538986	2757924	26.04%	4.622%
8	9.308	1092	1101	1112	rBV	1467134	2693701	25.43%	4.515%
9	10.965	1376	1383	1394	rBV	638405	1176097	11.10%	1.971%
10	13.409	1791	1799	1809	rBV	4150399	6379642	60.24%	10.693%
11	14.237	1932	1940	1946	rBV	802384	1258360	11.88%	2.109%
12	14.795	2028	2035	2044	rVB2	1103471	1874197	17.70%	3.141%
13	15.612	2170	2174	2181	rVB	80317	115284	1.09%	0.193%
14	16.287	2282	2289	2307	rBV	4360472	6779282	64.01%	11.363%
15	16.475	2316	2321	2333	rBV	114021	230570	2.18%	0.386%
16	17.274	2452	2457	2463	rBV2	72495	110294	1.04%	0.185%
17	17.550	2496	2504	2513	rBV2	1663269	2643704	24.96%	4.431%
18	18.419	2645	2652	2663	rBV	272900	479023	4.52%	0.803%
19	19.688	2864	2868	2873	rBV4	94795	128015	1.21%	0.215%
20	20.158	2942	2948	2958	rBV	7685016	10591004	100.00%	17.751%
21	21.474	3167	3172	3182	rBV4	151278	386892	3.65%	0.648%
22	21.868	3231	3239	3246	rBV2	1604047	2839309	26.81%	4.759%
23	25.251	3804	3815	3827	rVB	906917	2604979	24.60%	4.366%

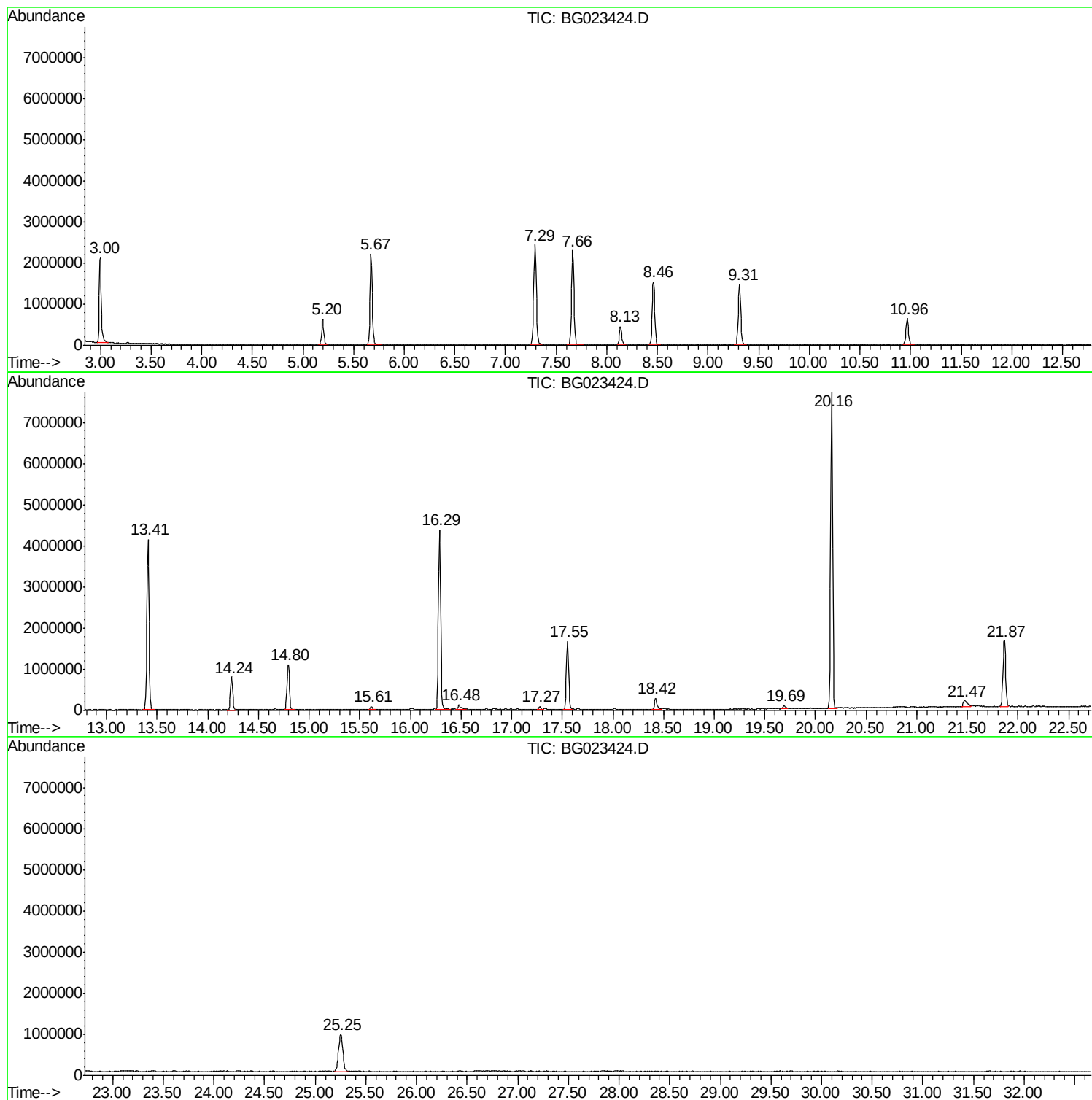
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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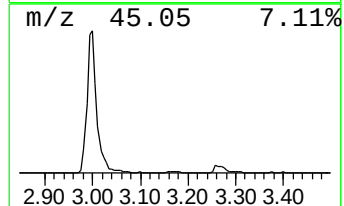
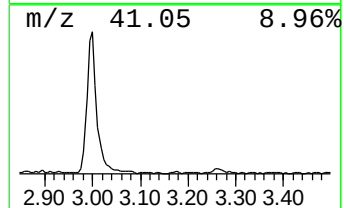
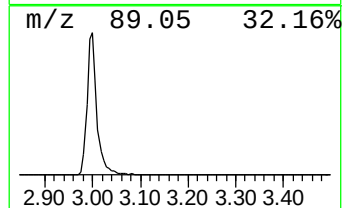
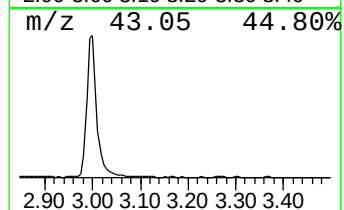
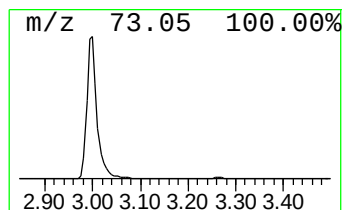
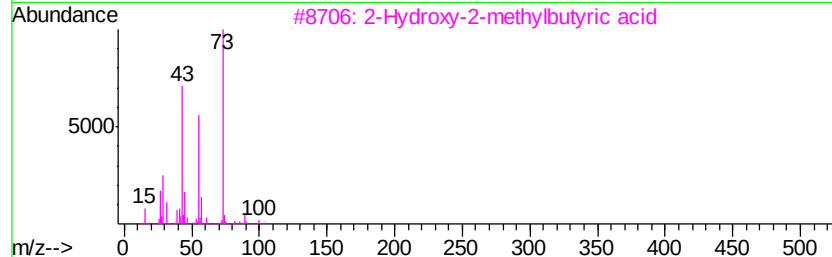
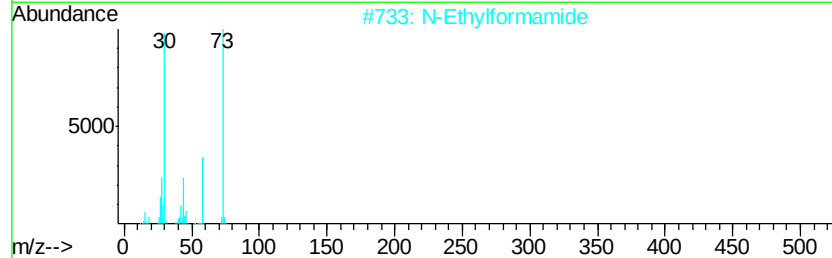
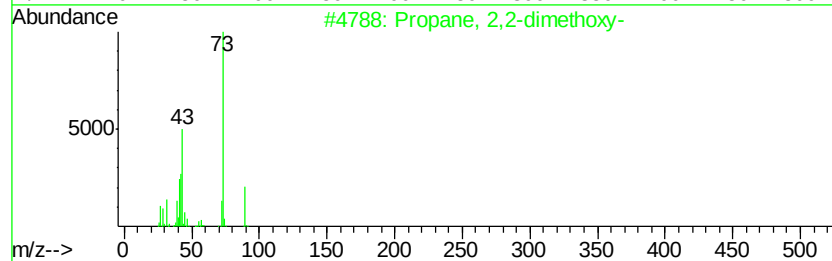
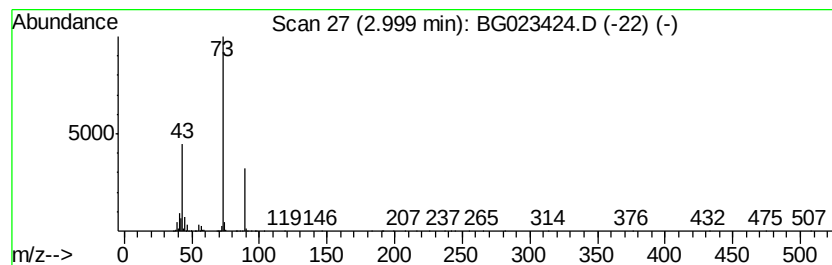
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	79.65 ng	3030630	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	56
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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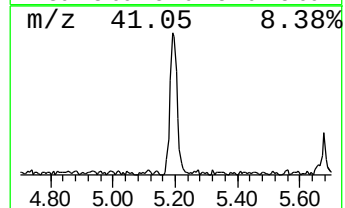
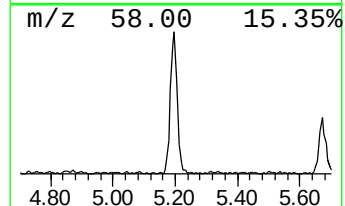
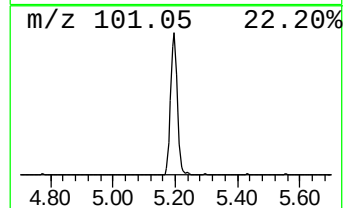
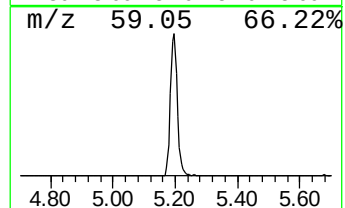
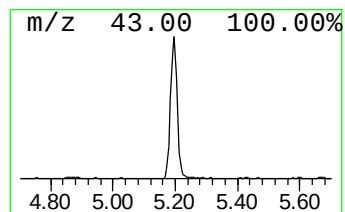
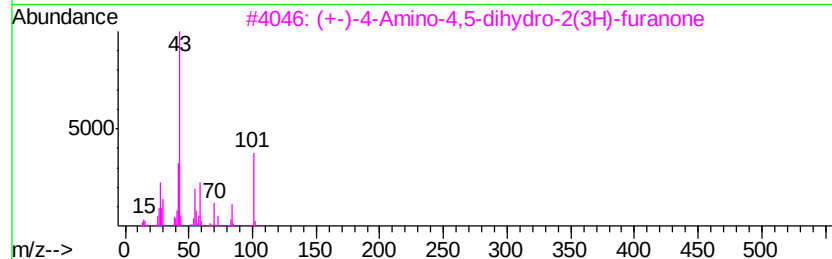
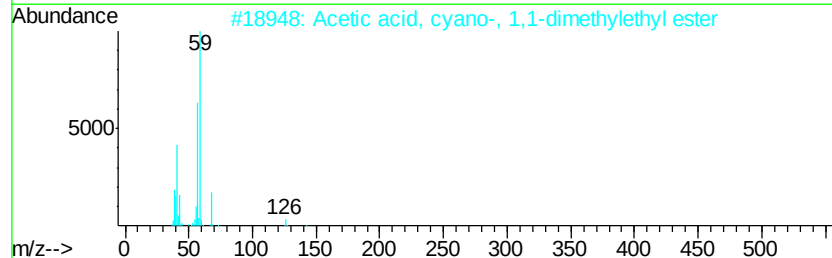
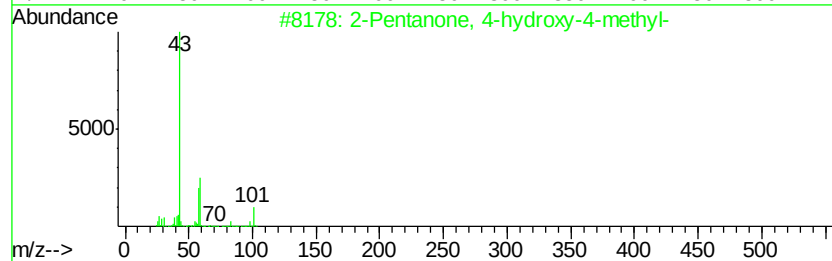
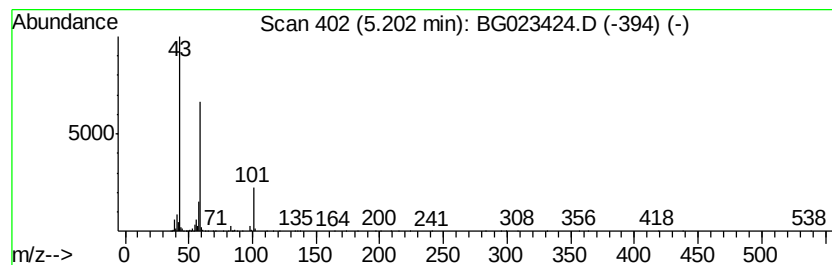
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	24.77 ng	942472	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
4		Acetone	58	C3H6O	000067-64-1	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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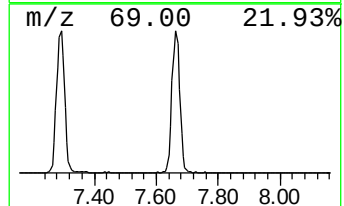
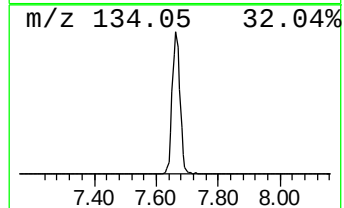
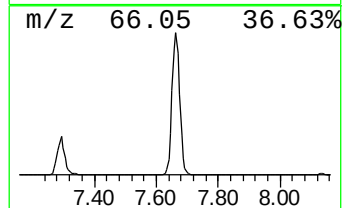
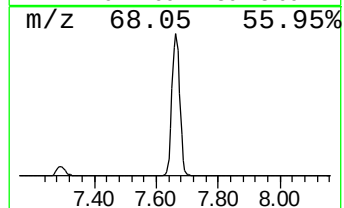
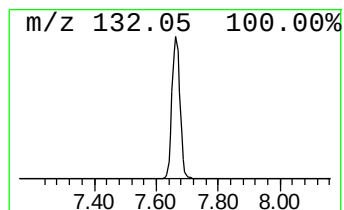
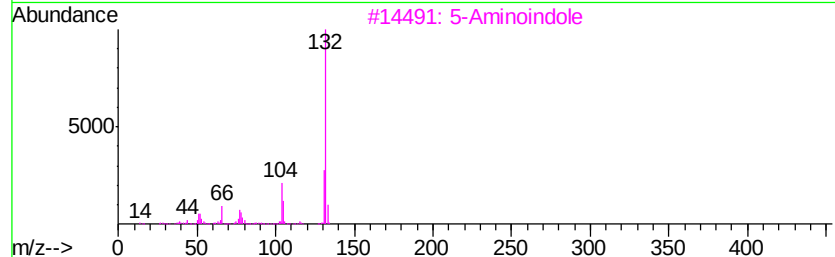
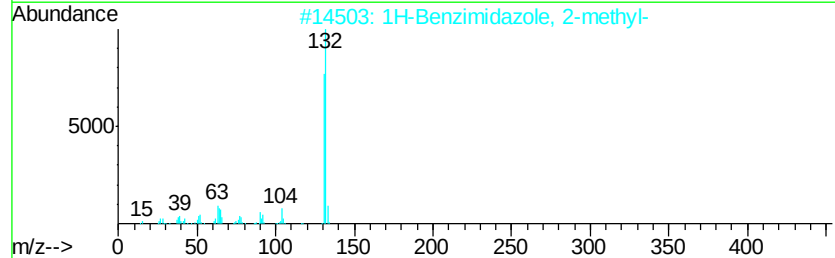
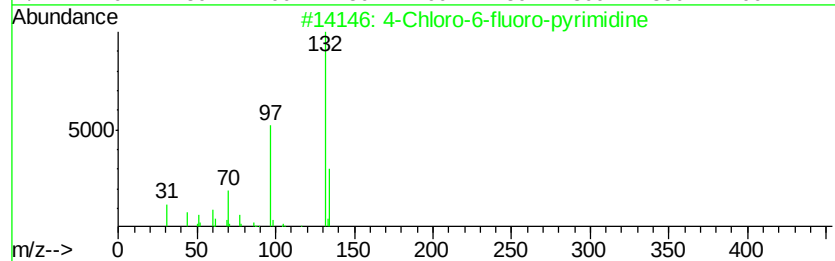
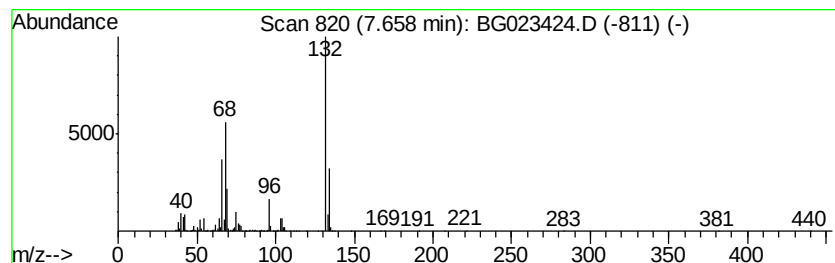
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Peak Number 3 unknown7.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	105.63 ng	4019180	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		2-Cyclohexen-1-one	96	C6H8O	000930-68-7	11



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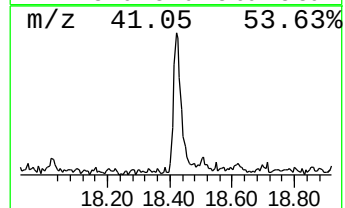
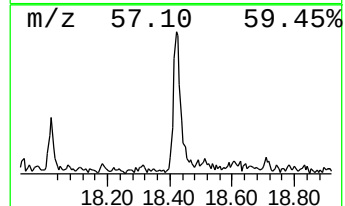
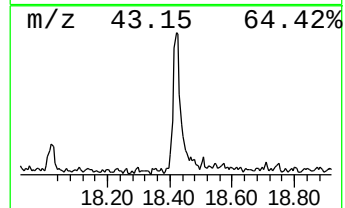
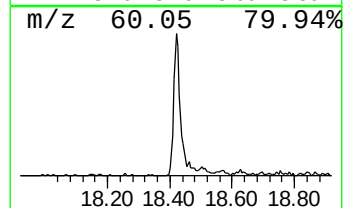
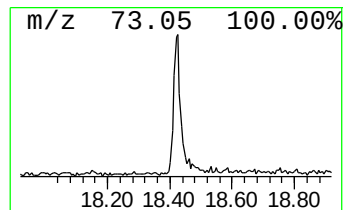
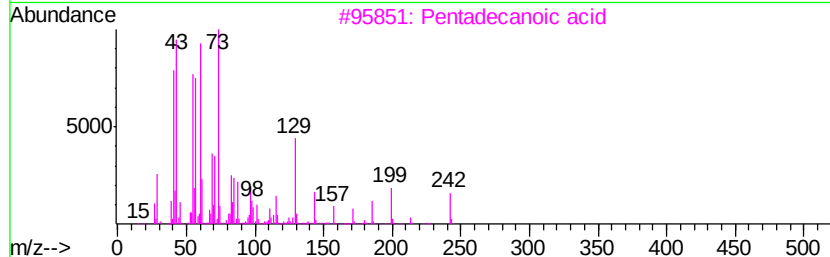
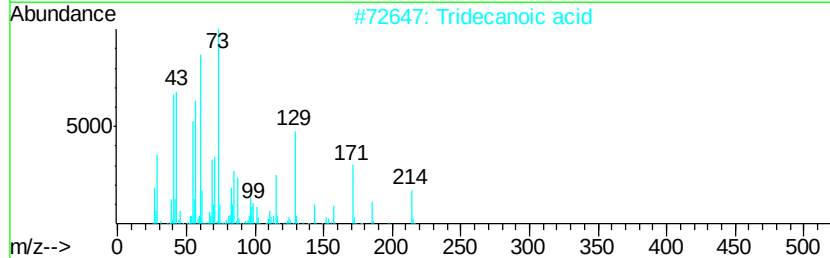
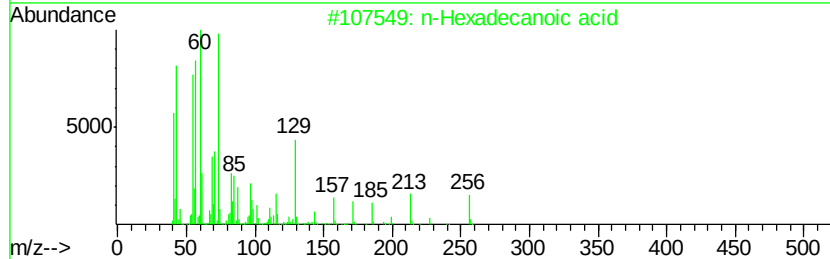
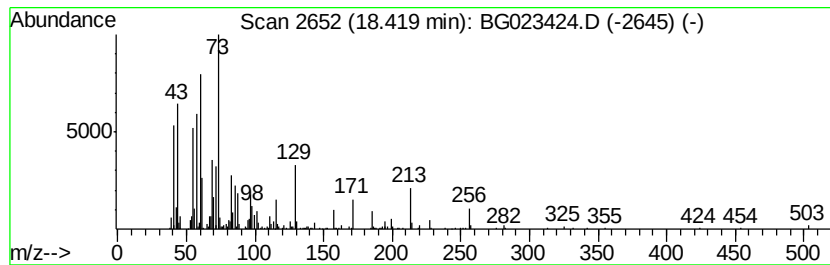
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	3.62 ng	479023	Phenanthrene-d10	17.55

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5	Dodecanoic acid	200	C12H24O2	000143-07-7	64



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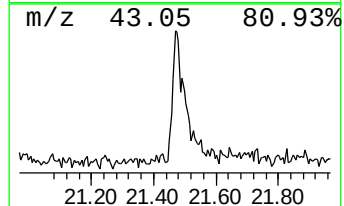
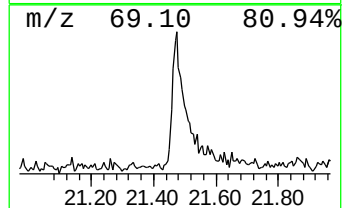
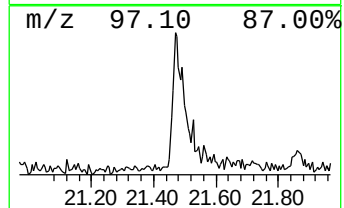
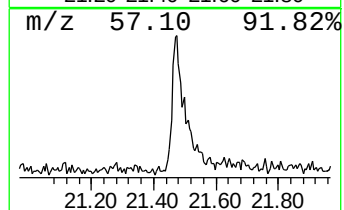
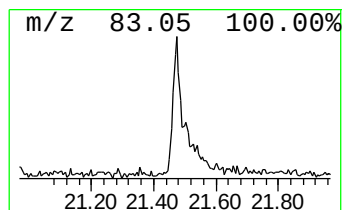
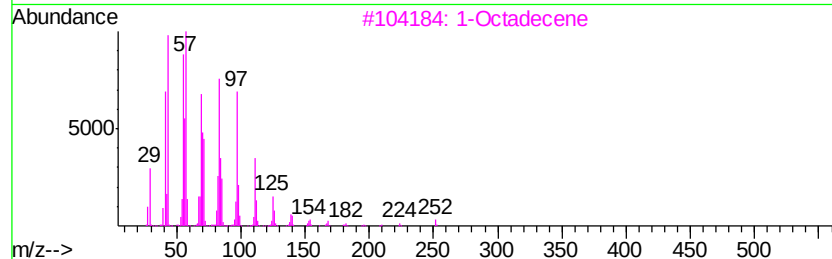
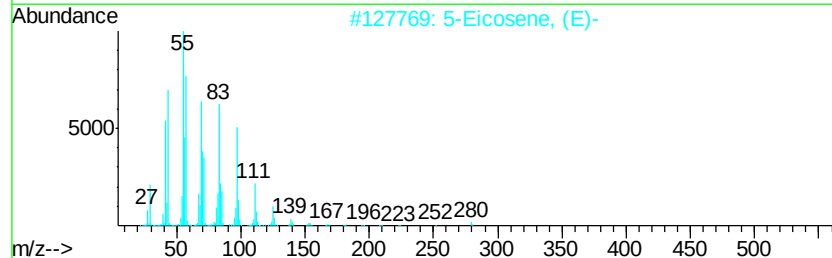
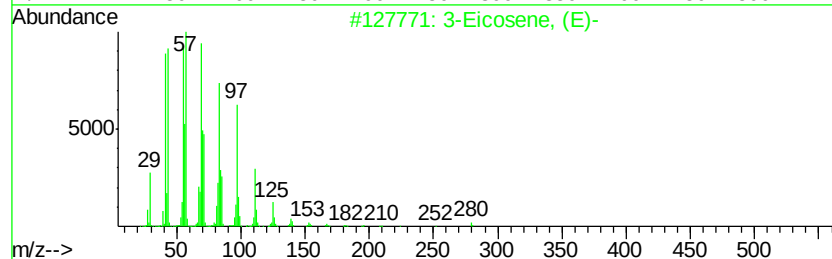
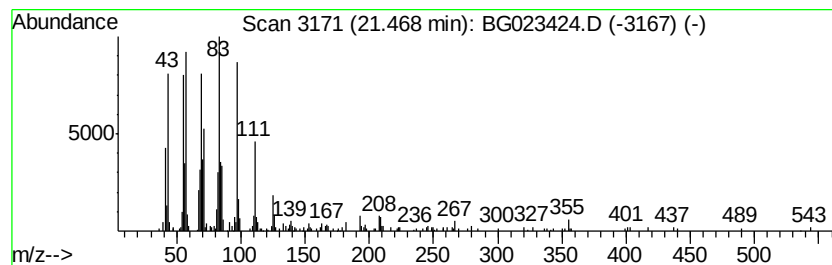
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Peak Number 6 3-Eicosene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.47	2.73 ng	386892	Chrysene-d12	21.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	1-Octadecene	252	C18H36	000112-88-9	90
4	1-Heptadecene	238	C17H34	006765-39-5	87
5	5-Octadecene, (E)-	252	C18H36	007206-21-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	3.00	79.7	ng	3030630	1	8.13	761008	20.0
2-Pentanone, 4-hy...	5.20	24.8	ng	942472	1	8.13	761008	20.0
unknown7.66	7.66	105.6	ng	4019180	1	8.13	761008	20.0
n-Hexadecanoic acid	18.42	3.6	ng	479023	4	17.55	2643700	20.0
3-Eicosene, (E)-	21.47	2.7	ng	386892	5	21.87	2839310	20.0