

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040918\
 Data File : BG033674.D
 Acq On : 9 Apr 2018 11:00
 Operator : SJ/JU
 Sample : J2258-01
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 11984

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.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	3.478	26	32	43	rBV	68517	149608	4.48%	0.797%
2	3.567	43	47	55	rVB	51202	81739	2.45%	0.435%
3	5.770	416	422	433	rVB2	45534	81544	2.44%	0.434%
4	6.281	502	509	524	rBV	779294	1499202	44.93%	7.983%
5	7.967	787	796	816	rBV	773269	1752450	52.52%	9.332%
6	8.373	857	865	887	rBV	758397	1574258	47.18%	8.383%
7	8.854	938	947	967	rBV2	116221	281678	8.44%	1.500%
8	9.189	996	1004	1015	rBV	544544	1064866	31.91%	5.670%
9	10.053	1141	1151	1172	rBV	427658	1004499	30.10%	5.349%
10	11.739	1431	1438	1452	rBV	177154	381461	11.43%	2.031%
11	14.101	1833	1840	1858	rBV	1045267	1798981	53.91%	9.579%
12	14.894	1966	1975	1983	rBV	84319	142877	4.28%	0.761%
13	15.300	2038	2044	2049	rBV2	30400	48707	1.46%	0.259%
14	15.476	2067	2074	2083	rBV2	334282	585388	17.54%	3.117%
15	15.752	2116	2121	2125	rBV	33553	51539	1.54%	0.274%
16	16.240	2199	2204	2209	rVB	41997	55611	1.67%	0.296%
17	16.945	2318	2324	2340	rBV	1143558	1913346	57.34%	10.188%
18	17.092	2345	2349	2358	rVB	42057	65966	1.98%	0.351%
19	18.202	2532	2538	2552	rBV	438473	786018	23.56%	4.185%
20	19.001	2669	2674	2686	rBV2	67659	126524	3.79%	0.674%
21	20.723	2961	2967	2977	rBV	2352214	3336867	100.00%	17.768%
22	22.068	3191	3196	3204	rBV5	44542	85826	2.57%	0.457%
23	22.550	3270	3278	3286	rBV2	483867	920333	27.58%	4.901%
24	25.124	3709	3716	3725	rVB3	31508	81841	2.45%	0.436%
25	26.305	3906	3917	3931	rVB3	250980	842517	25.25%	4.486%
26	27.580	4127	4134	4144	rBV8	20255	66069	1.98%	0.352%

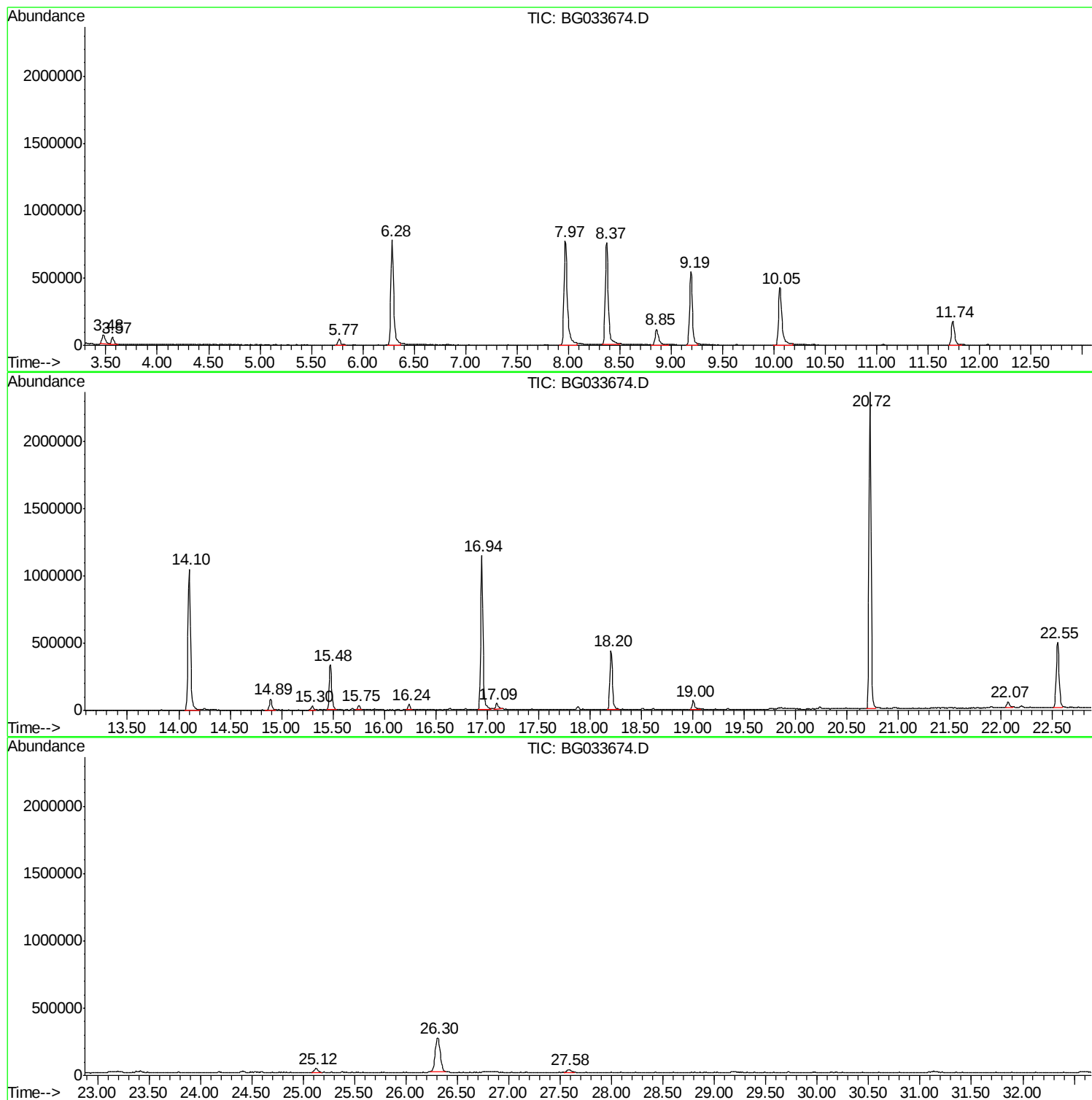
Sum of corrected areas: 18779715

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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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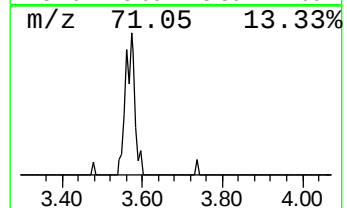
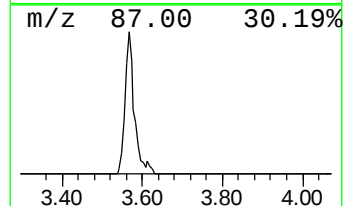
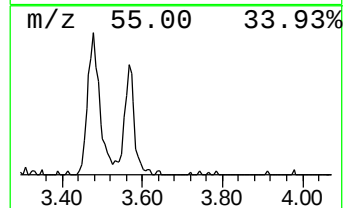
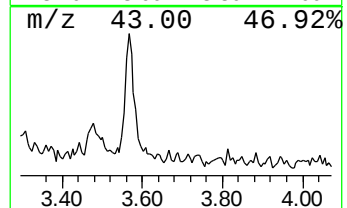
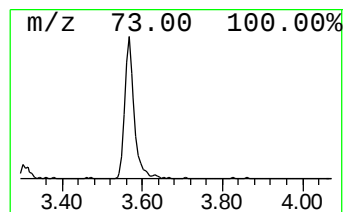
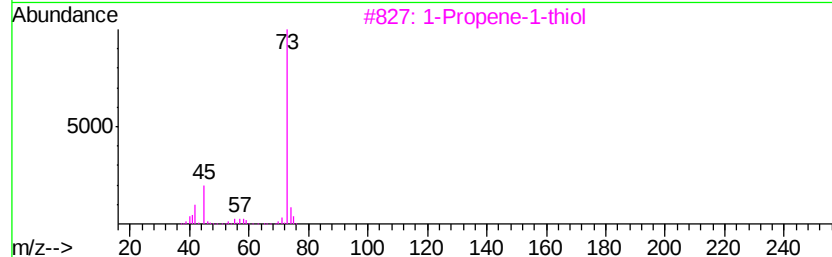
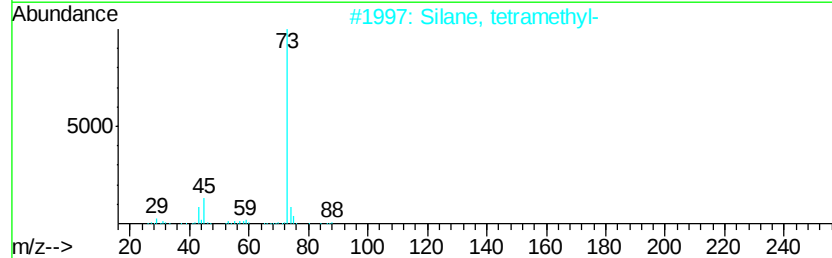
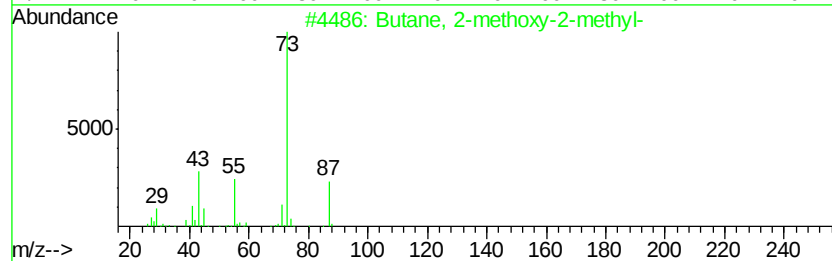
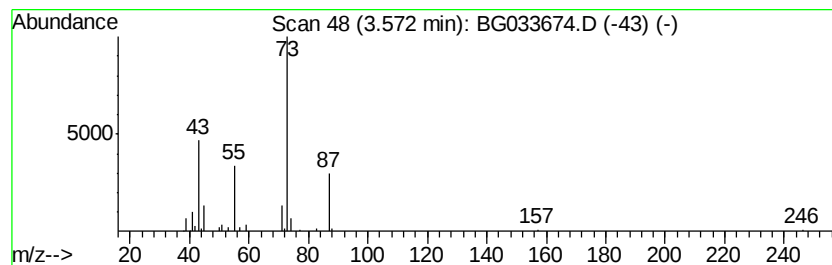
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	5.80 ng	81739	1,4-Dichlorobenzene-d4	8.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			Silane, tetramethyl-	88	C4H12Si	000075-76-3	43
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	43
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5			Boronic acid, ethyl-, dimethyl e...	102	C4H11B02	007318-82-3	9



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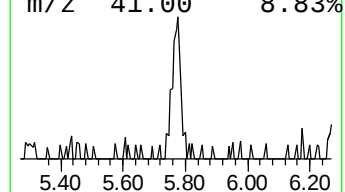
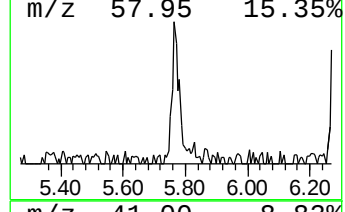
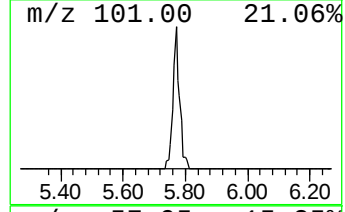
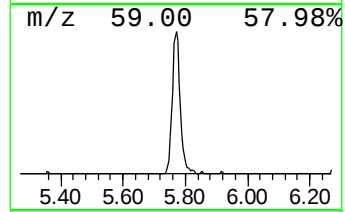
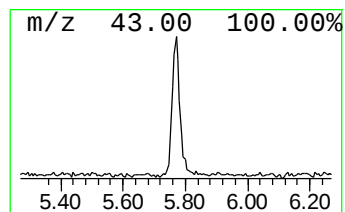
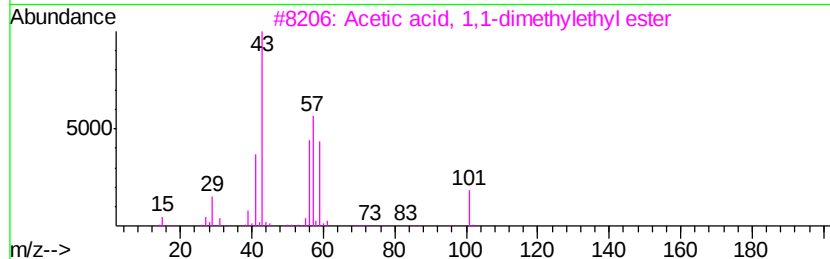
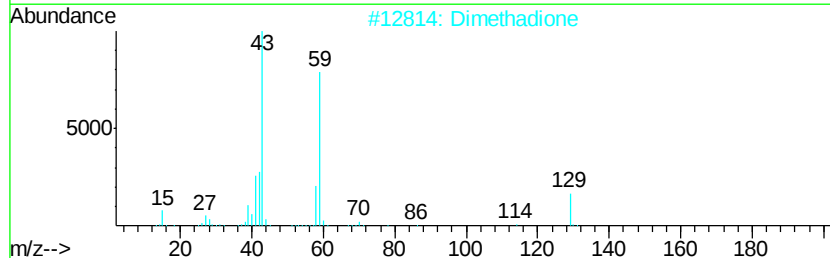
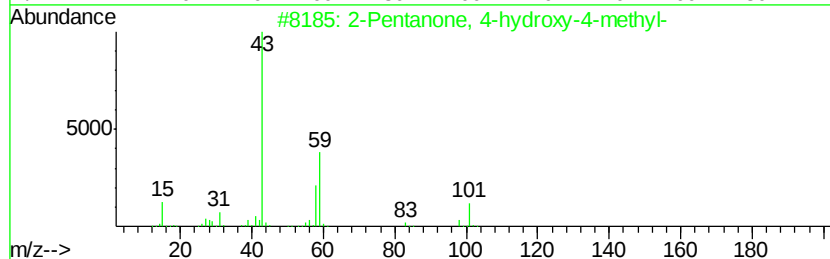
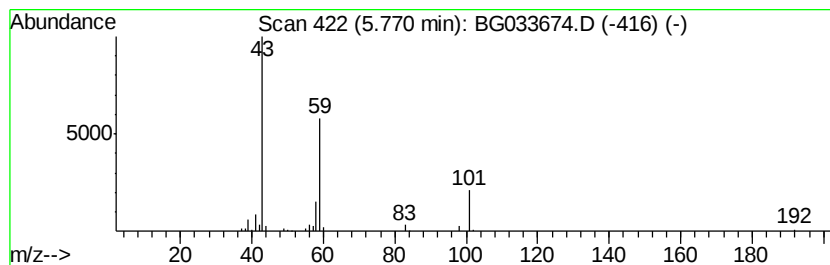
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.77	5.79 ng	81544	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Dimethadione	129	C5H7NO3	000695-53-4	40
3		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
5		3-Hexanol	102	C6H14O	000623-37-0	23



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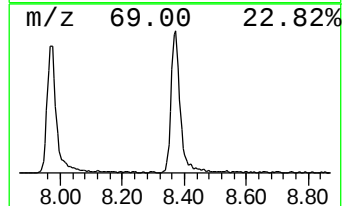
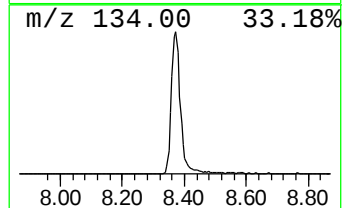
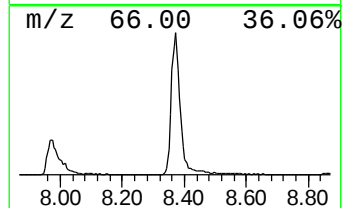
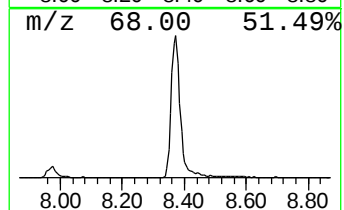
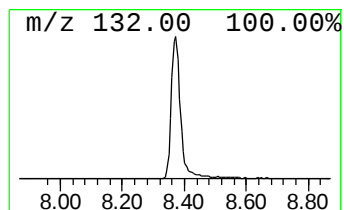
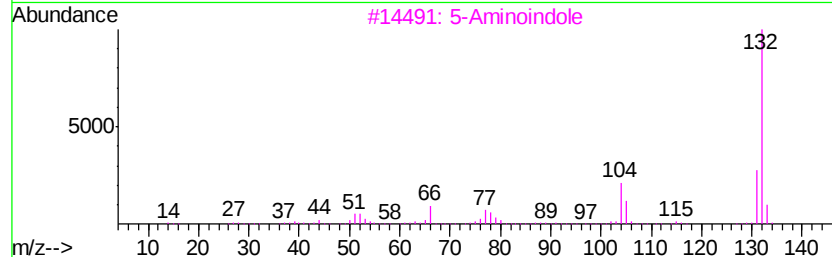
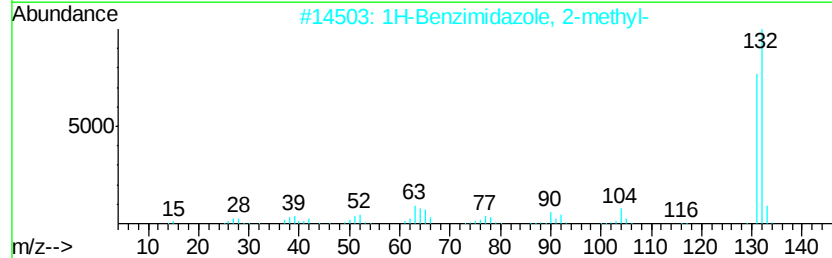
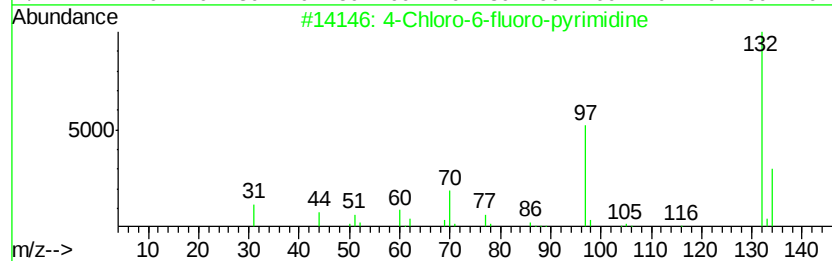
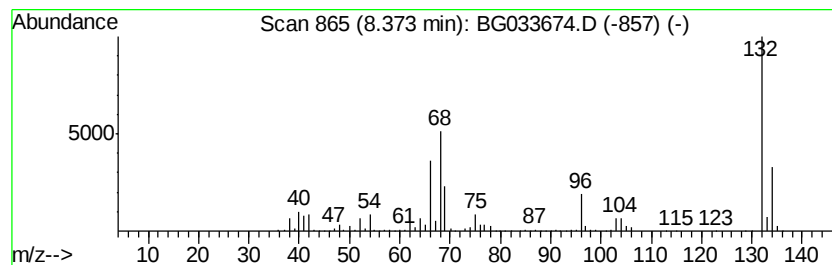
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Peak Number 4 unknown8.37 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.37	111.78 ng	1574260	1,4-Dichlorobenzene-d4	8.86

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	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	22
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17



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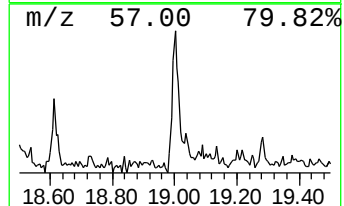
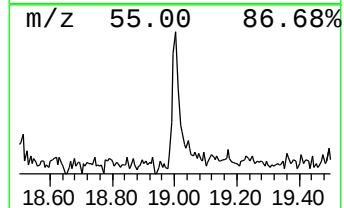
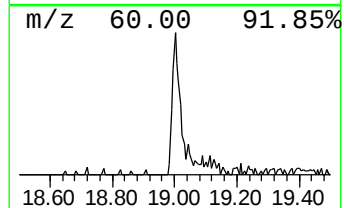
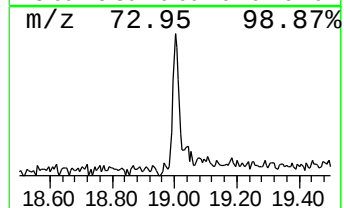
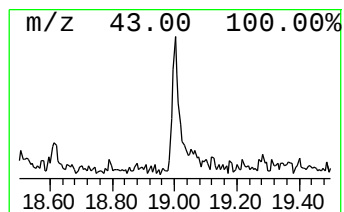
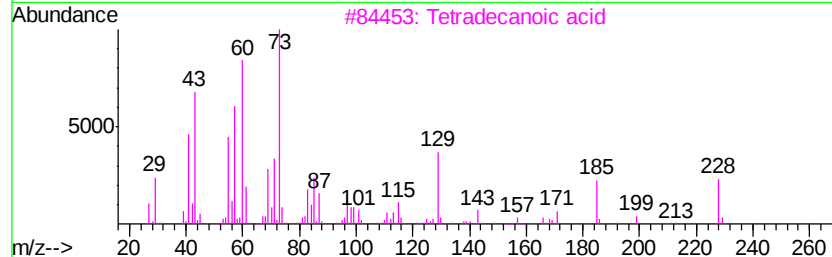
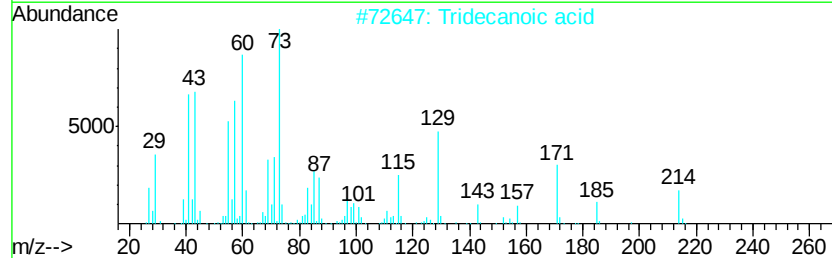
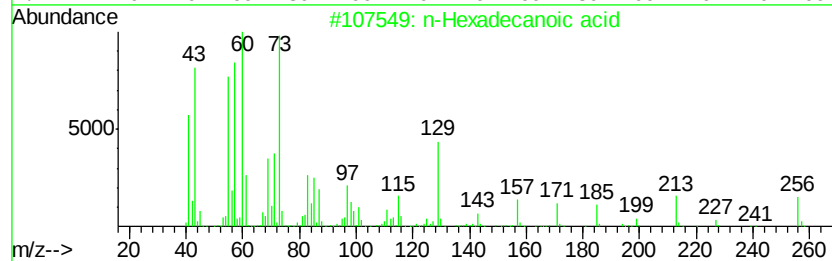
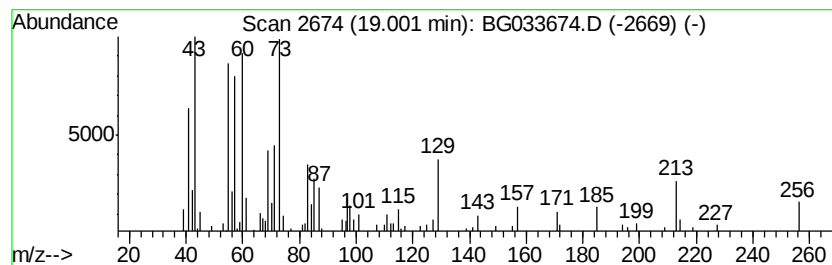
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.00	3.22 ng	126524	Phenanthrene-d10	18.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tridecanoic acid	214	C13H26O2	000638-53-9	80
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5		n-Decanoic acid	172	C10H20O2	000334-48-5	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	5.8	ng	81739	1	8.86	281678	20.0
2-Pentanone, 4-hy...	5.77	5.8	ng	81544	1	8.86	281678	20.0
unknown8.37	8.37	111.8	ng	1574260	1	8.86	281678	20.0
n-Hexadecanoic acid	19.00	3.2	ng	126524	4	18.20	786018	20.0