

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_G\DATA\BG011518\
 Data File : BG032044.D
 Acq On : 15 Jan 2018 22:36
 Operator : SJ/JU
 Sample : J1117-21
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COMP-3

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-BG011218.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	3.408	14	20	30	rBV2	44940	93049	2.16%	0.465%
2	3.496	30	35	46	rVB	40628	63563	1.47%	0.318%
3	5.682	400	407	418	rVB	36447	63340	1.47%	0.317%
4	6.193	486	494	504	rBV	698678	1209776	28.04%	6.047%
5	7.874	772	780	792	rBV	693277	1292192	29.95%	6.459%
6	8.279	841	849	858	rBV	734650	1350922	31.31%	6.753%
7	8.767	921	932	942	rVB2	138627	252938	5.86%	1.264%
8	9.102	980	989	1004	rBV	559654	1052788	24.40%	5.262%
9	9.965	1127	1136	1145	rBV	404219	775536	17.97%	3.877%
10	11.652	1414	1423	1431	rBV	191797	357821	8.29%	1.789%
11	14.025	1818	1827	1839	rBV	1341017	2123574	49.22%	10.615%
12	14.824	1956	1963	1969	rBV	120900	188514	4.37%	0.942%
13	15.400	2053	2061	2070	rVB2	343418	575126	13.33%	2.875%
14	16.875	2304	2312	2324	rBV	1442298	2317817	53.72%	11.586%
15	18.132	2515	2526	2537	rBV2	558024	881332	20.43%	4.405%
16	18.943	2659	2664	2676	rBV2	101460	182252	4.22%	0.911%
17	20.664	2951	2957	2967	rBV	3289032	4314617	100.00%	21.567%
18	22.004	3179	3185	3198	rBV	171170	307154	7.12%	1.535%
19	22.292	3228	3234	3242	rBV	165746	271624	6.30%	1.358%
20	22.468	3256	3264	3276	rBV	618583	1148684	26.62%	5.742%
21	26.182	3883	3896	3912	rBV2	341311	1183375	27.43%	5.915%

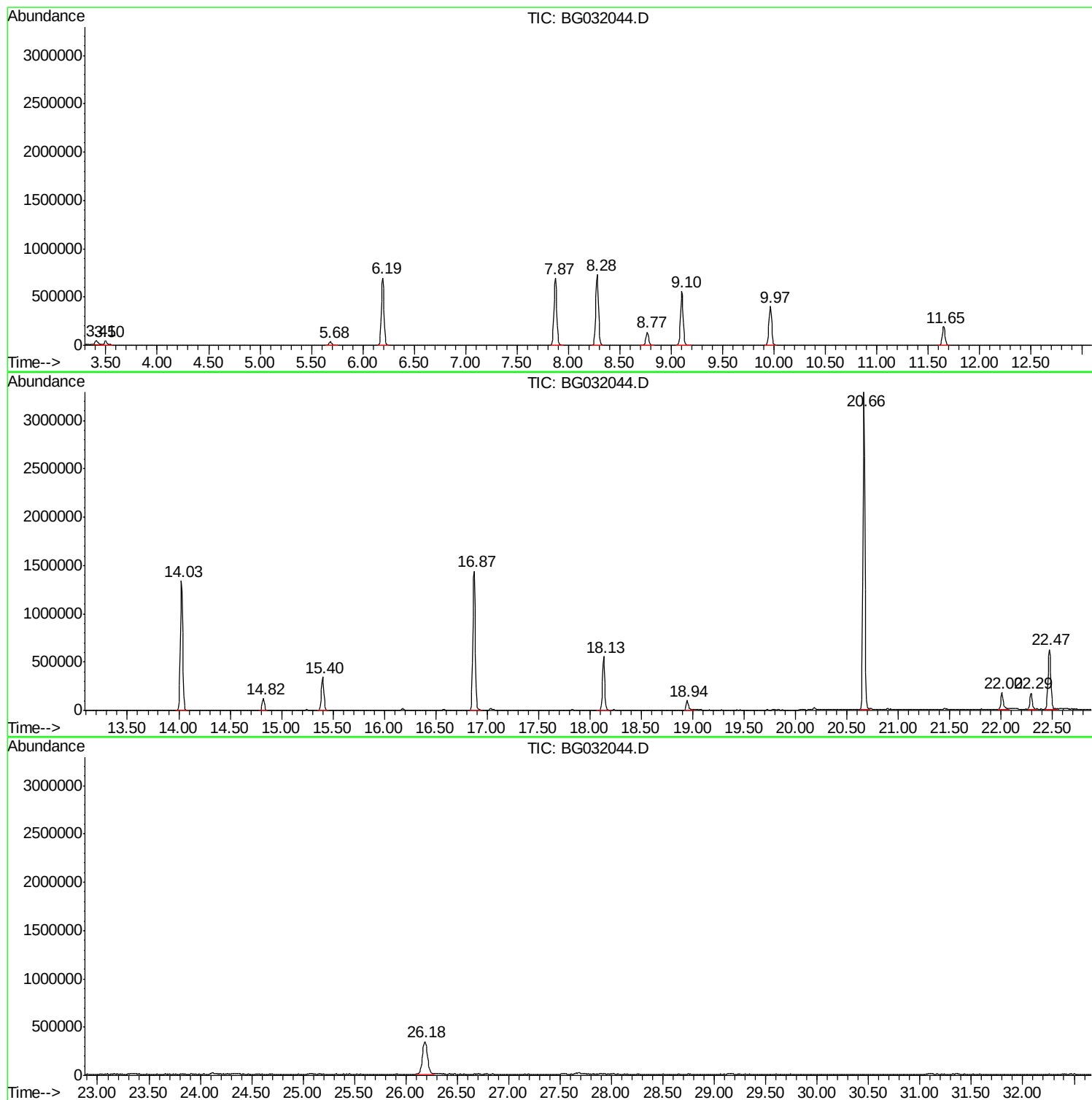
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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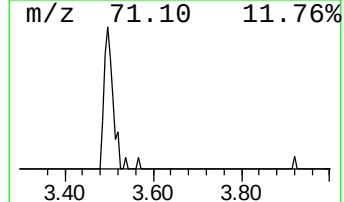
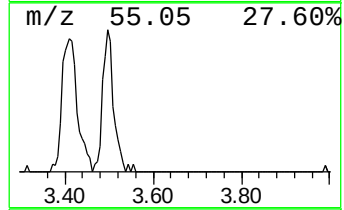
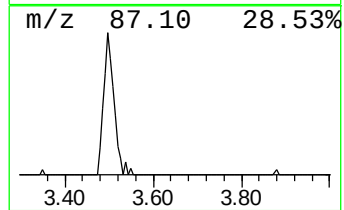
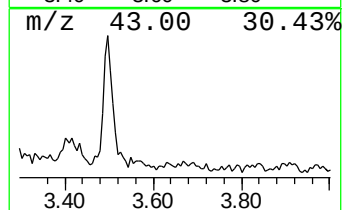
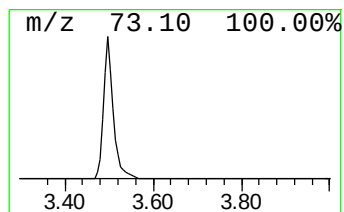
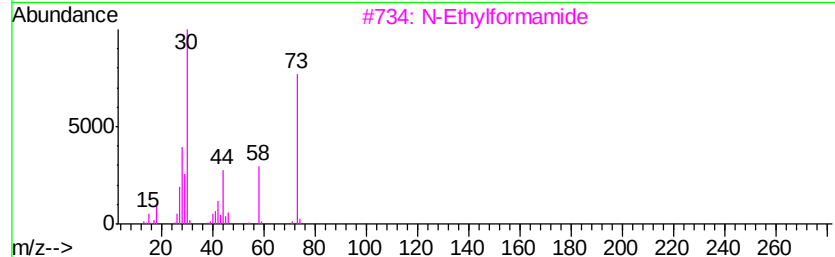
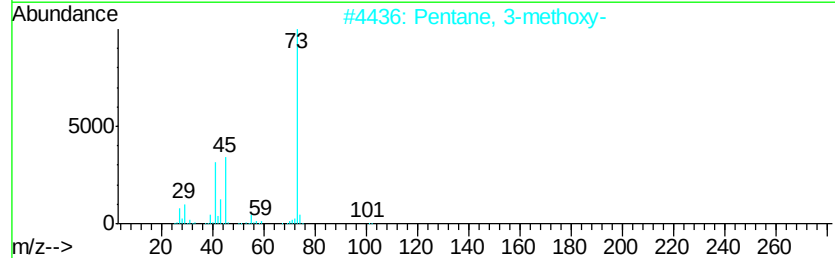
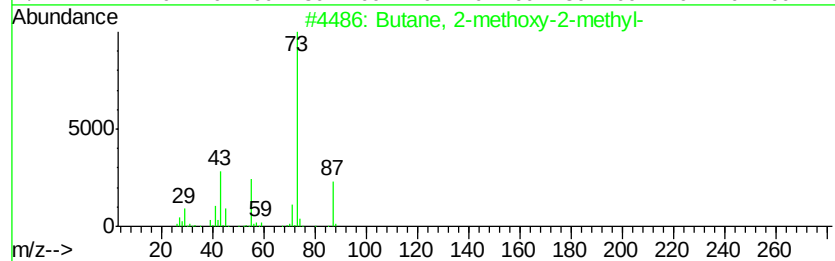
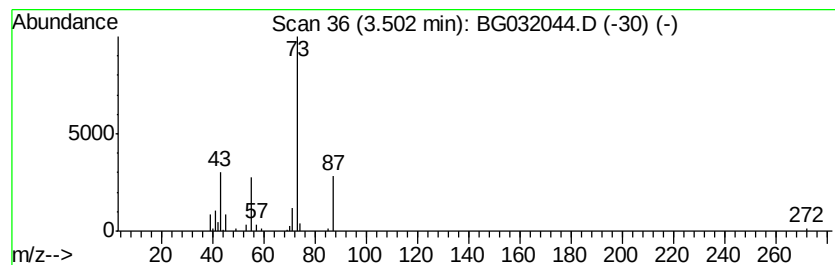
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG011218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.50	5.03 ng	63563	1,4-Dichlorobenzene-d4	8.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5



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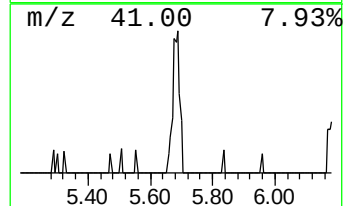
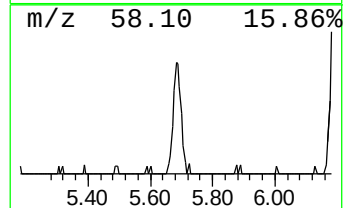
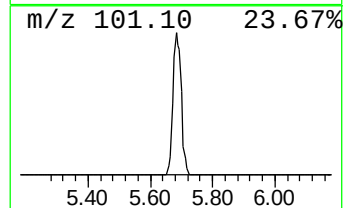
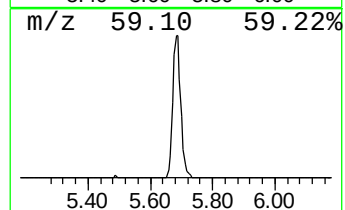
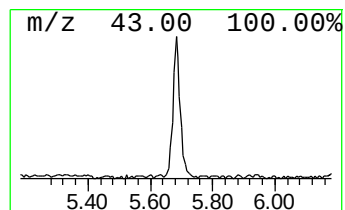
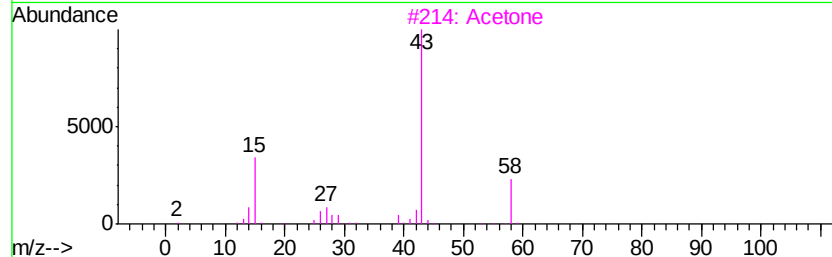
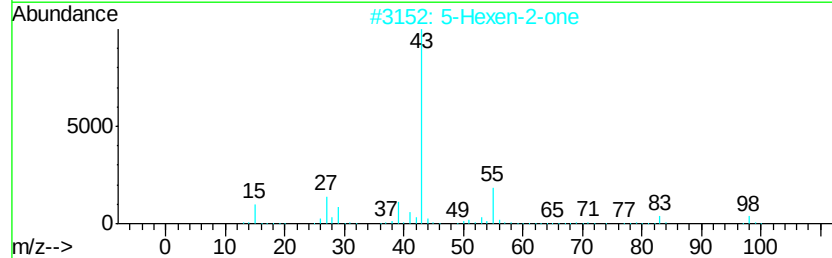
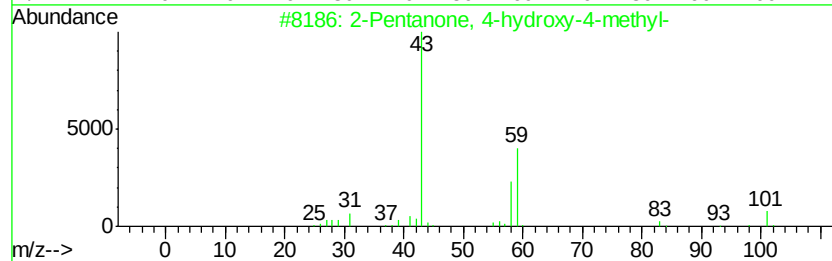
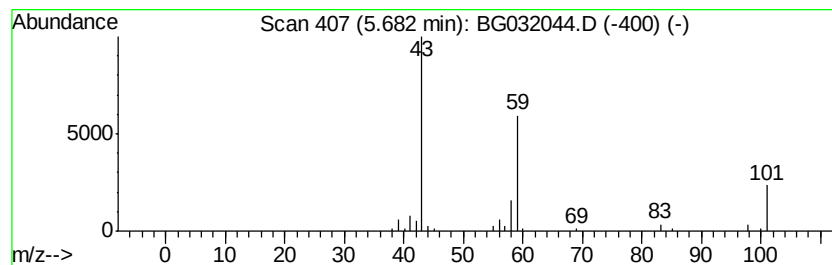
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.68	5.01 ng	63340	1,4-Dichlorobenzene-d4	8.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56	
2	5-Hexen-2-one	98	C6H10O	000109-49-9	9	
3	Acetone	58	C3H6O	000067-64-1	9	
4	Guanidine	59	CH5N3	000113-00-8	9	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	



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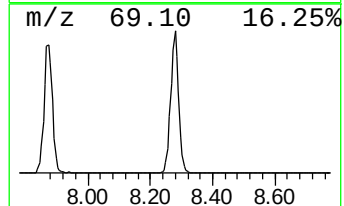
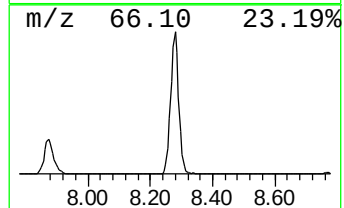
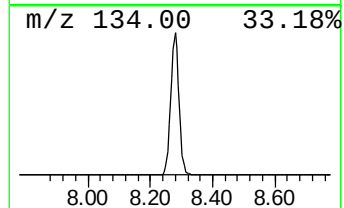
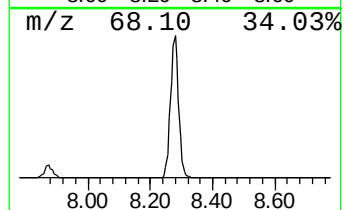
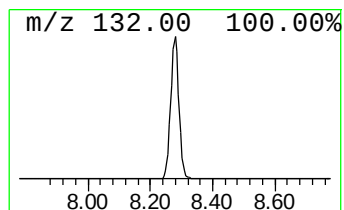
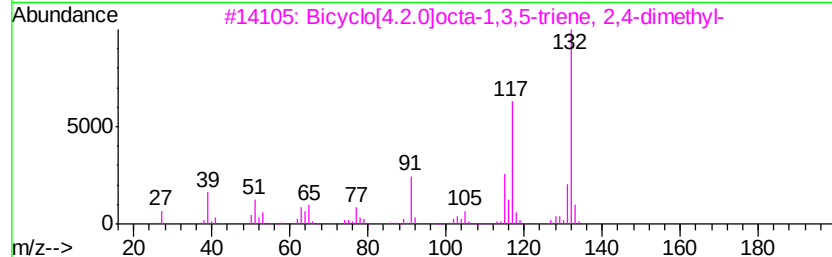
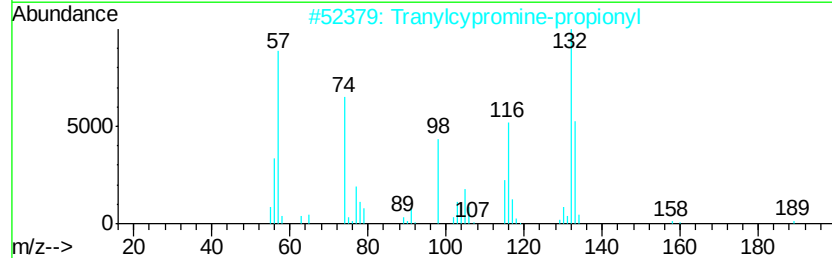
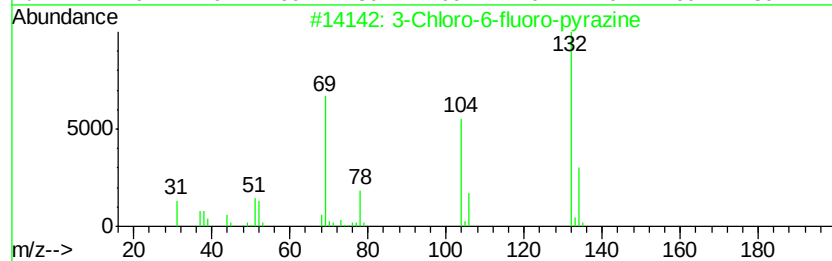
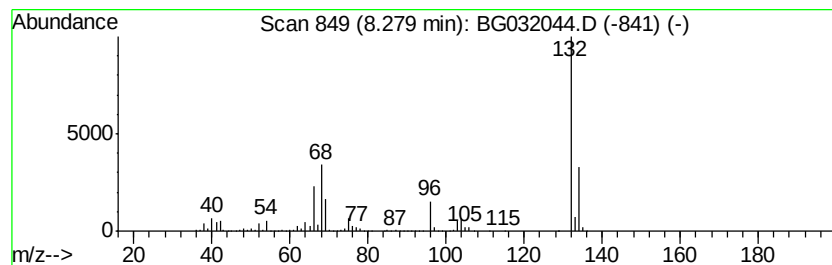
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Peak Number 4 unknown8.28 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.28	106.82 ng	1350920	1,4-Dichlorobenzene-d4	8.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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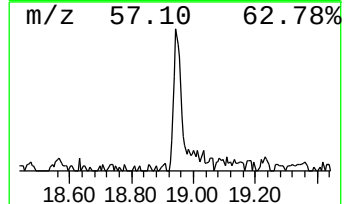
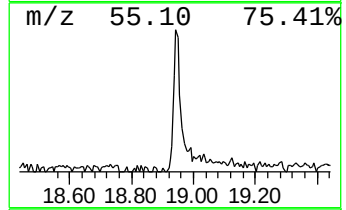
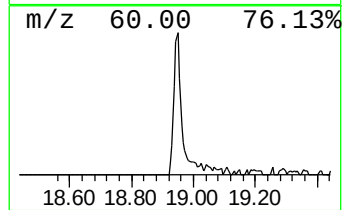
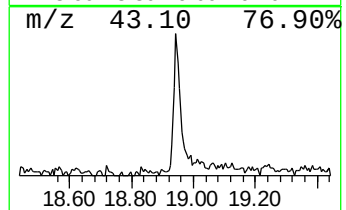
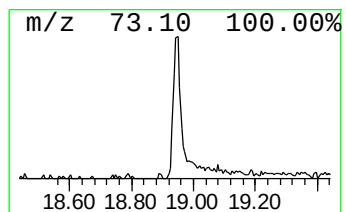
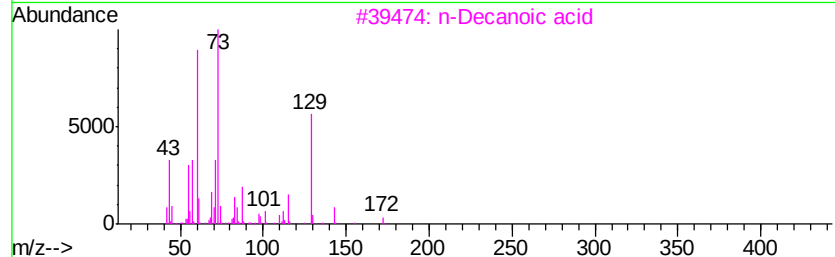
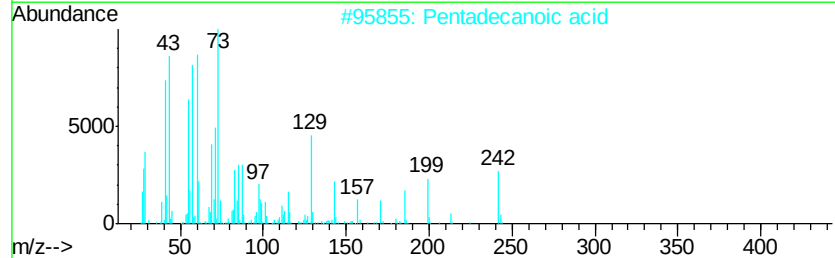
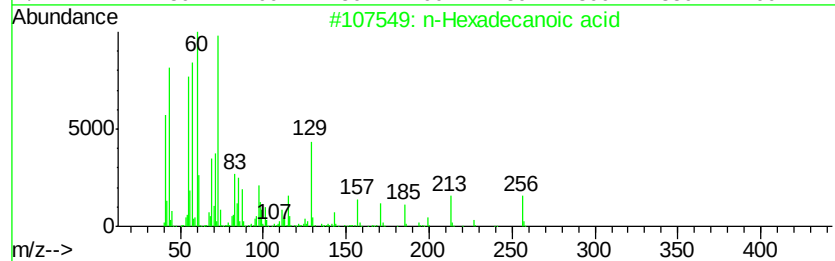
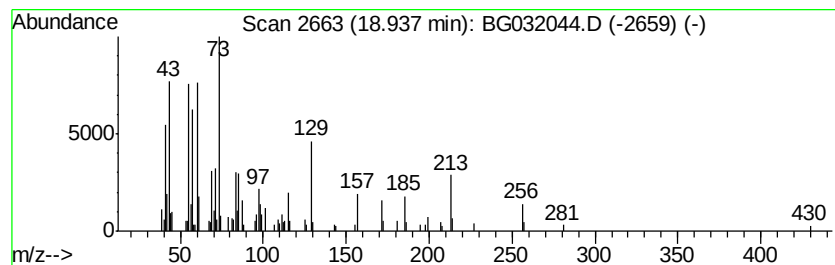
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.94	4.14 ng	182252	Phenanthrene-d10	18.13

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	47
3		n-Decanoic acid	172	C10H20O2	000334-48-5	38
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	35
5		Undecanoic acid	186	C11H22O2	000112-37-8	30



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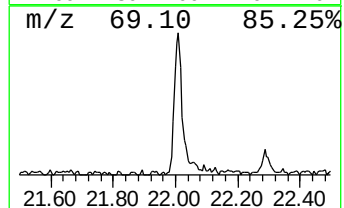
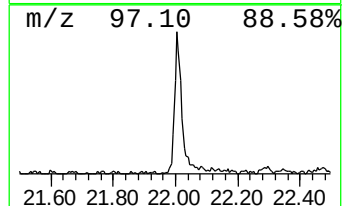
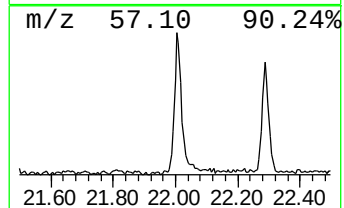
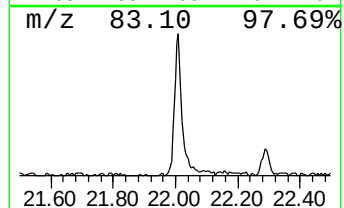
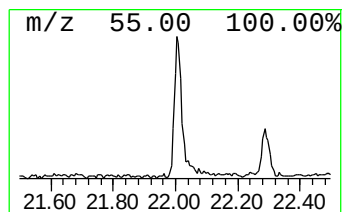
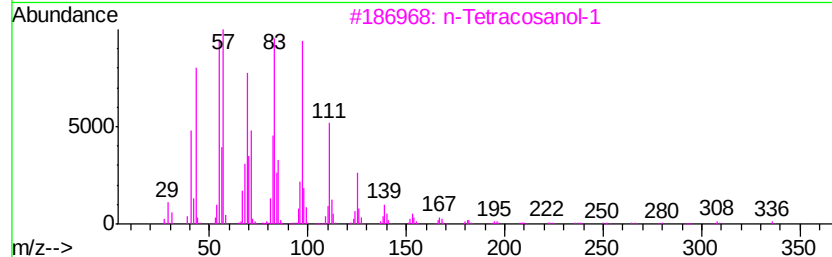
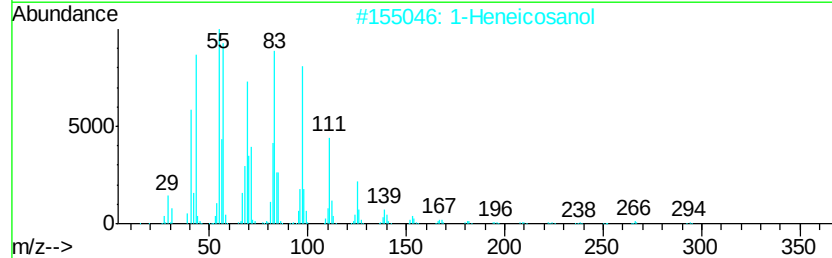
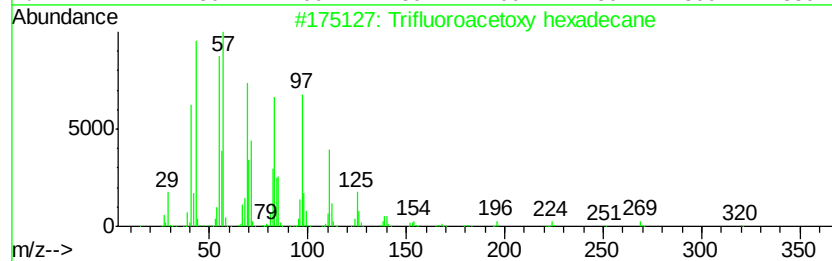
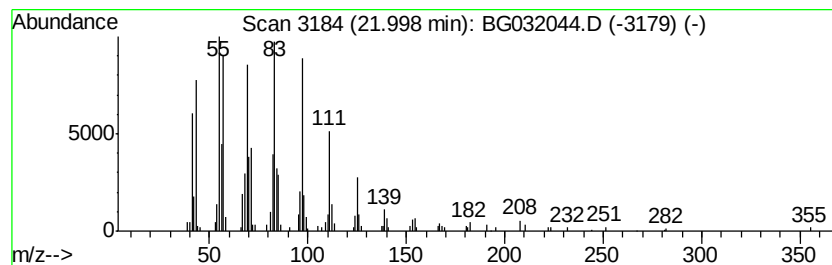
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Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.00	5.35 ng	307154	Chrysene-d12	22.47

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	93
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	93
5		1-Heptacosanol	396	C27H56O	002004-39-9	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.50	5.0	ng	63563	1	8.77	252938	20.0
2-Pentanone, 4-hy...	5.68	5.0	ng	63340	1	8.77	252938	20.0
unknown8.28	8.28	106.8	ng	1350920	1	8.77	252938	20.0
n-Hexadecanoic acid	18.94	4.1	ng	182252	4	18.13	881332	20.0
Trifluoroacetoxy ...	22.00	5.3	ng	307154	5	22.47	1148680	20.0