

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG082718\
Data File : BG036437.D
Acq On : 27 Aug 2018 18:39
Operator : JU/SJ
Sample : J4648-06
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-3-@-8-FT

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_G\METHODS\8270-BG082318.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	5.174	316	321	328	rBV	39269	60973	2.20%	0.330%
2	5.632	392	399	412	rVB	921986	1456931	52.56%	7.884%
3	7.218	660	669	686	rBV	960646	1648708	59.47%	8.922%
4	7.594	724	733	743	rBV	887615	1500315	54.12%	8.119%
5	8.064	805	813	821	rBV	208834	351027	12.66%	1.900%
6	8.388	859	868	877	rBV	578642	1001088	36.11%	5.417%
7	9.222	1002	1010	1019	rBV	511845	932527	33.64%	5.046%
8	10.873	1284	1291	1300	rVB	283050	515510	18.60%	2.790%
9	13.317	1699	1707	1714	rBV	1146072	1784520	64.37%	9.657%
10	14.140	1840	1847	1852	rBV	204230	303891	10.96%	1.645%
11	14.686	1933	1940	1950	rVB2	461223	739355	26.67%	4.001%
12	16.173	2186	2193	2205	rBV	1137980	1700910	61.36%	9.205%
13	17.430	2401	2407	2416	rBV2	641359	963932	34.77%	5.216%
14	18.323	2551	2559	2566	rBV2	64069	103984	3.75%	0.563%
15	20.039	2845	2851	2857	rBV	2141895	2772147	100.00%	15.002%
16	21.355	3069	3075	3084	rBV2	65663	143503	5.18%	0.777%
17	21.696	3126	3133	3143	rBV2	709478	1170230	42.21%	6.333%
18	21.913	3166	3170	3174	rVB3	22073	28310	1.02%	0.153%
19	22.530	3270	3275	3280	rBV5	19313	32918	1.19%	0.178%
20	23.223	3388	3393	3399	rVB4	18871	32082	1.16%	0.174%
21	23.417	3420	3426	3431	rVB	24536	43204	1.56%	0.234%
22	24.034	3527	3531	3537	rVB5	18591	34975	1.26%	0.189%
23	24.915	3670	3681	3691	rBV3	387961	1119547	40.39%	6.059%
24	26.143	3883	3890	3898	rVB7	13274	38266	1.38%	0.207%

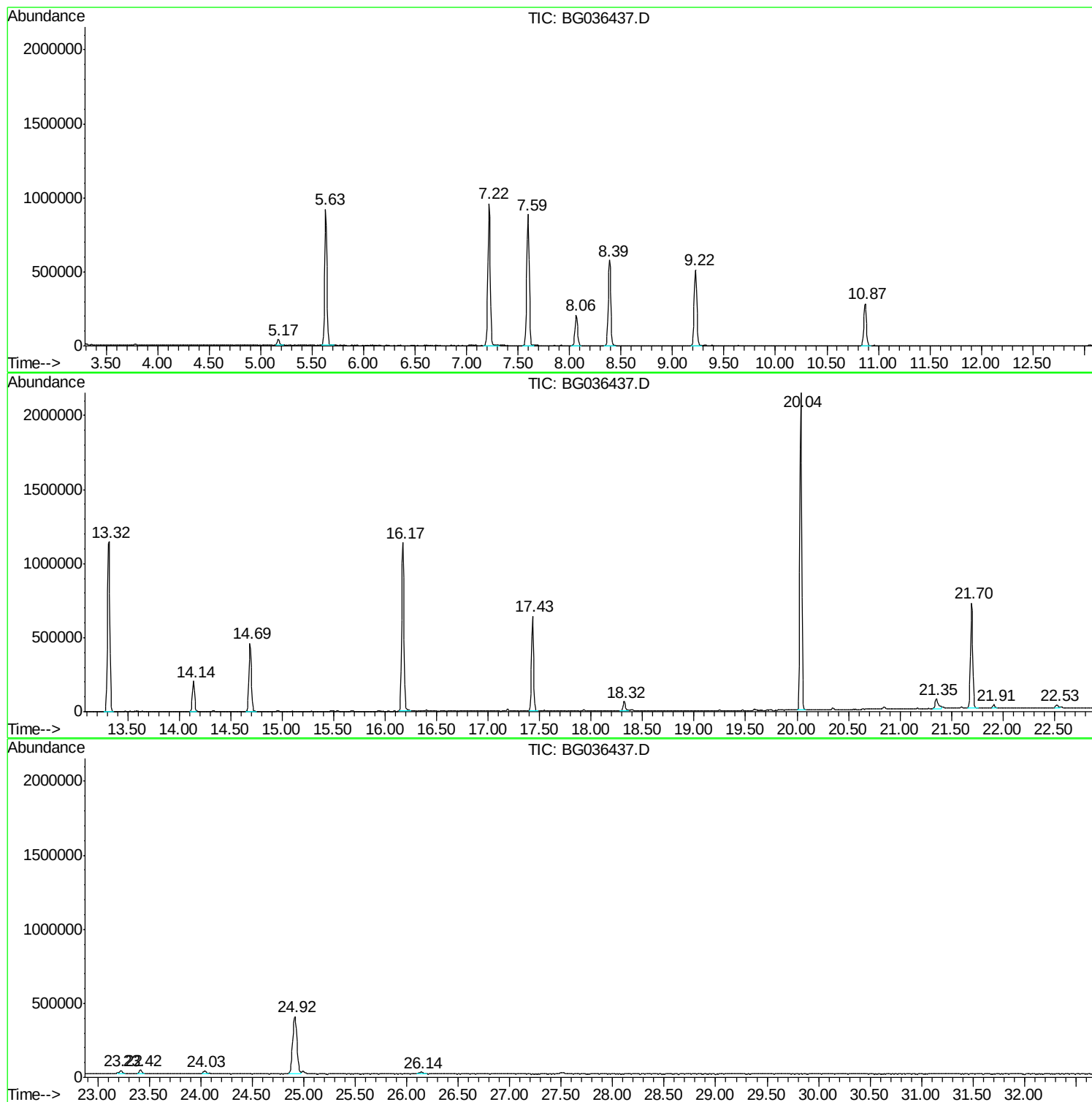
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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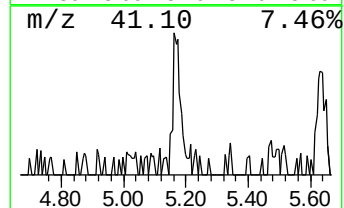
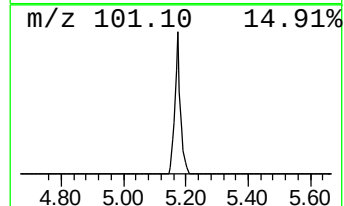
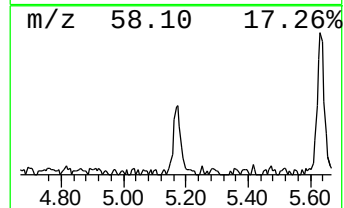
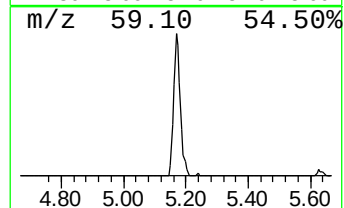
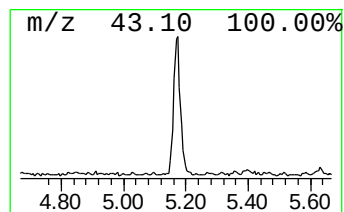
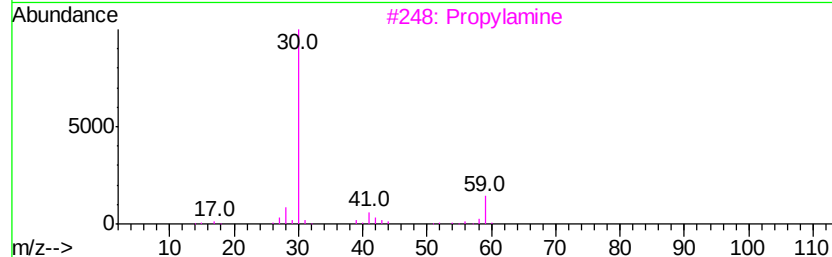
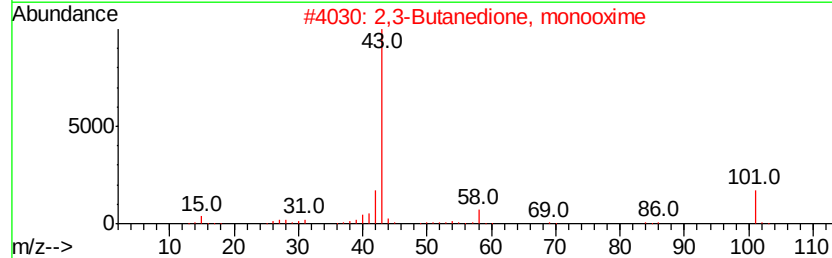
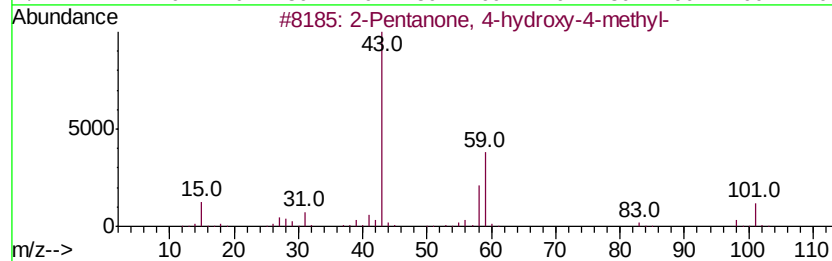
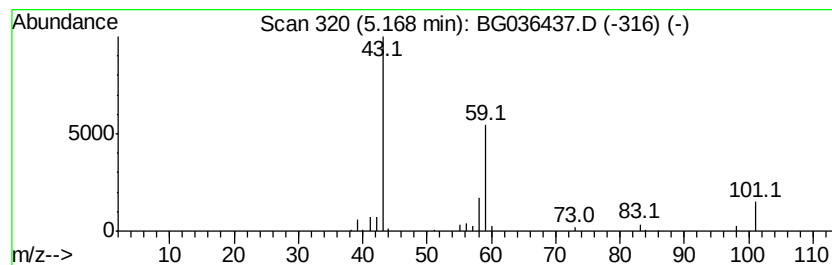
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	3.47 ng	60973	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3			Propylamine	59	C3H9N	000107-10-8	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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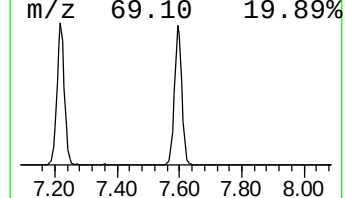
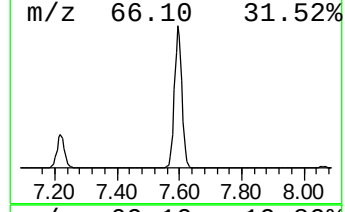
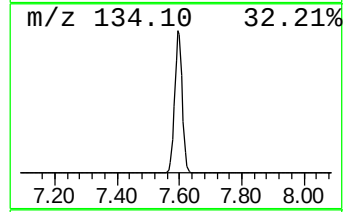
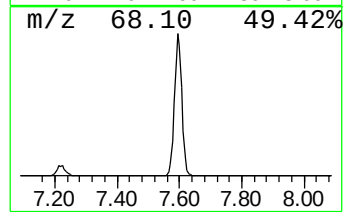
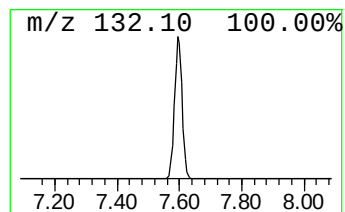
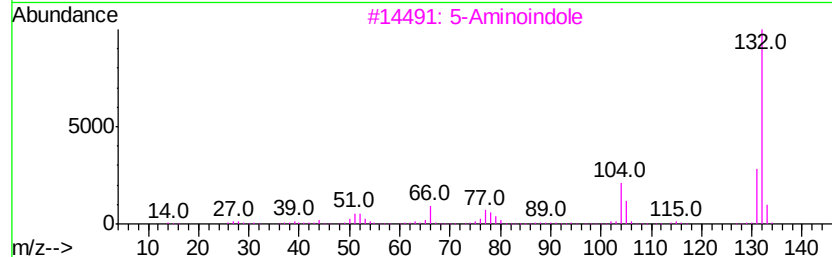
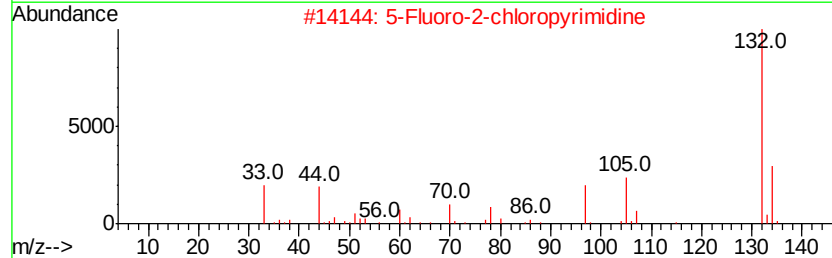
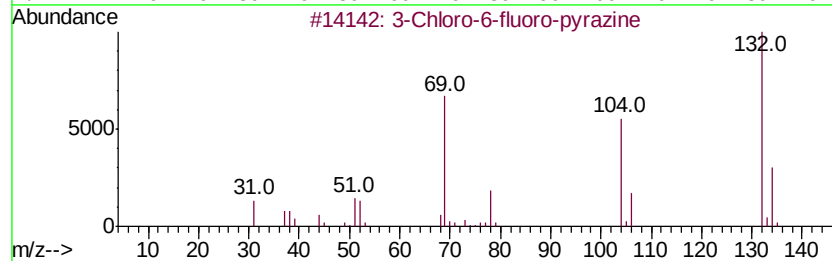
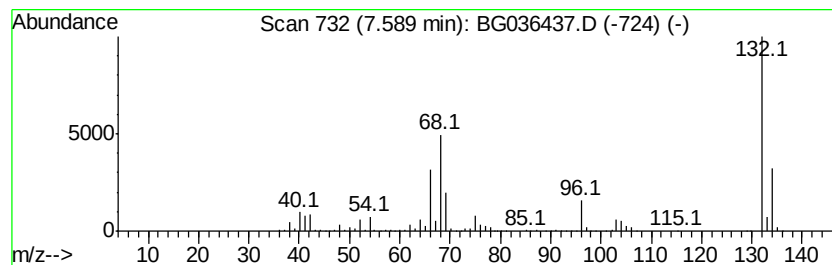
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Peak Number 2 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	85.48 ng	1500320	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



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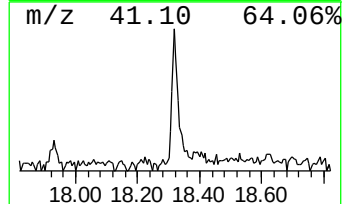
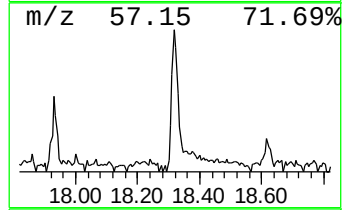
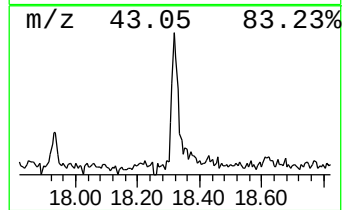
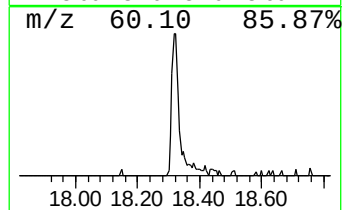
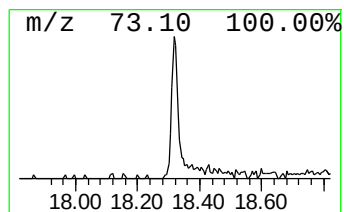
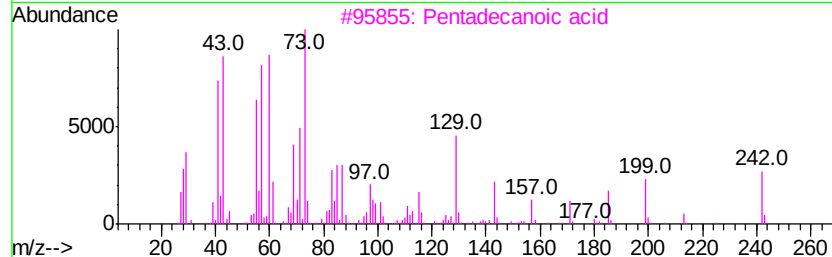
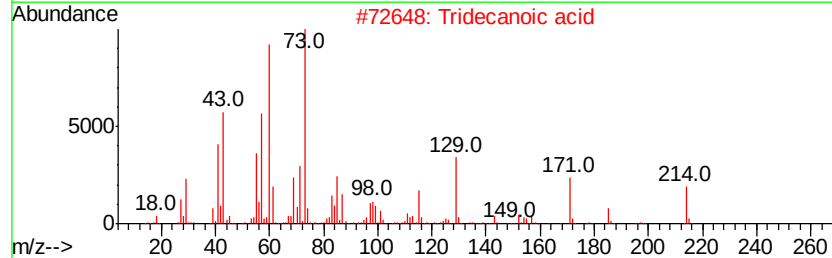
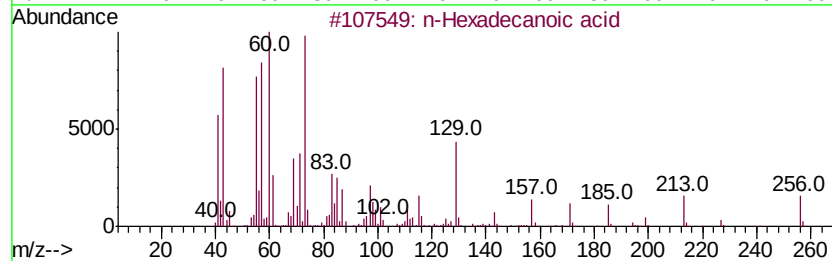
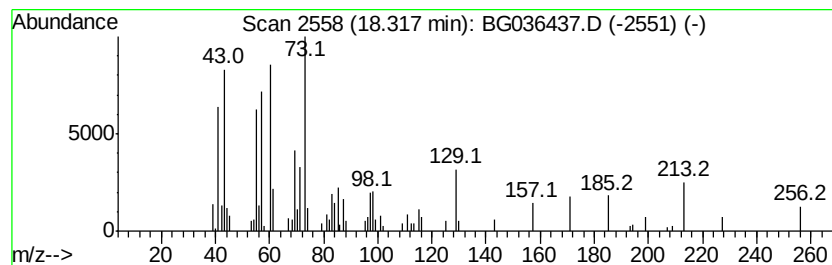
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.32	2.16 ng	103984	Phenanthrene-d10	17.43

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	58
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	53
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	Dodecanoic acid	200	C12H24O2	000143-07-7	52



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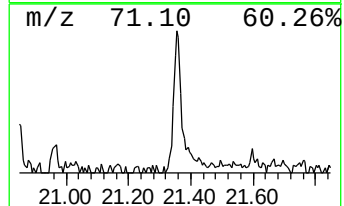
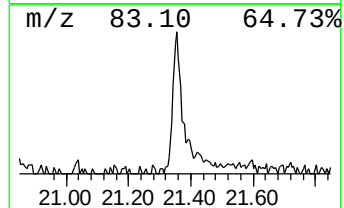
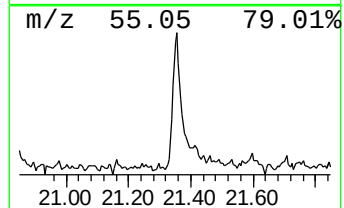
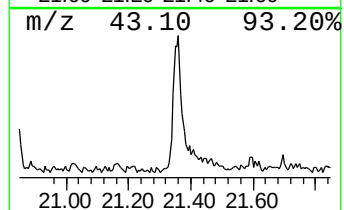
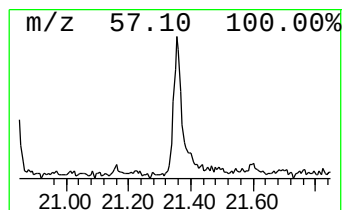
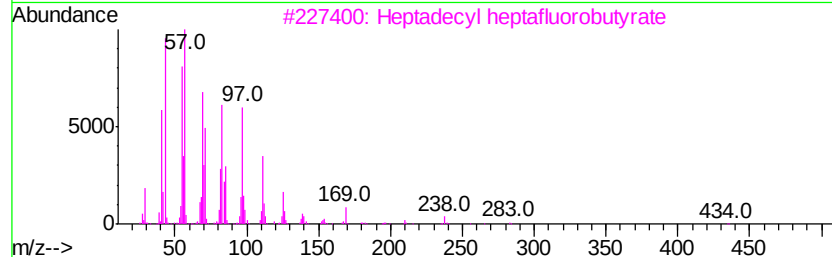
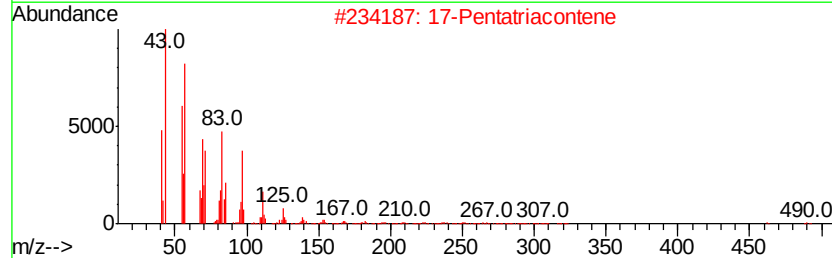
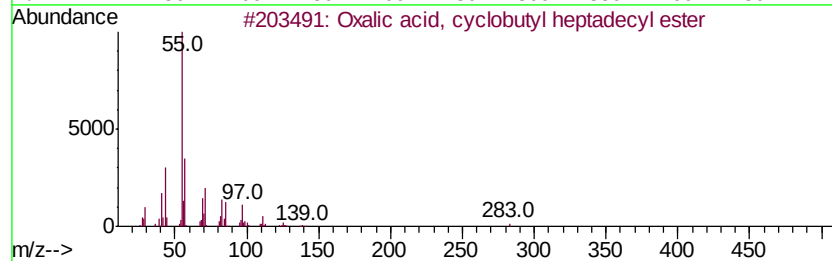
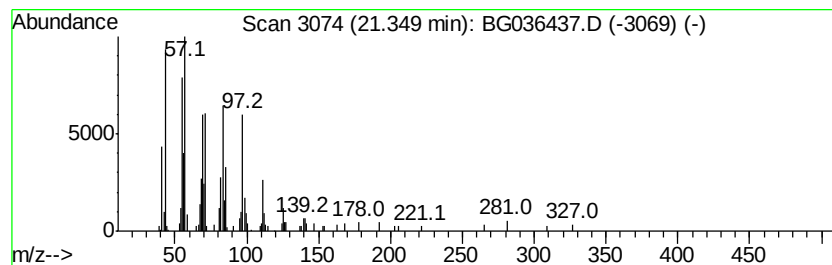
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Peak Number 5 Oxalic acid, cyclobutyl hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.35	2.45 ng	143503	Chrysene-d12	21.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, cyclobutyl heptadec...	382	C23H42O4	1000309-70-7	87
2		17-Pentatriacontene	491	C35H70	006971-40-0	83
3		Heptadecyl heptafluorobutvrate	452	C21H35F7O2	959085-66-6	81
4		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	81
5		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.17	3.5	ng	60973	1	8.06	351027	20.0
unknown7.59	7.59	85.5	ng	1500320	1	8.06	351027	20.0
n-Hexadecanoic acid	18.32	2.2	ng	103984	4	17.43	963932	20.0
Oxalic acid, cycl...	21.35	2.5	ng	143503	5	21.70	1170230	20.0