

Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG101518\
 Data File : BG037340.D
 Acq On : 15 Oct 2018 19:20
 Operator : JU/SJ
 Sample : J5461-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

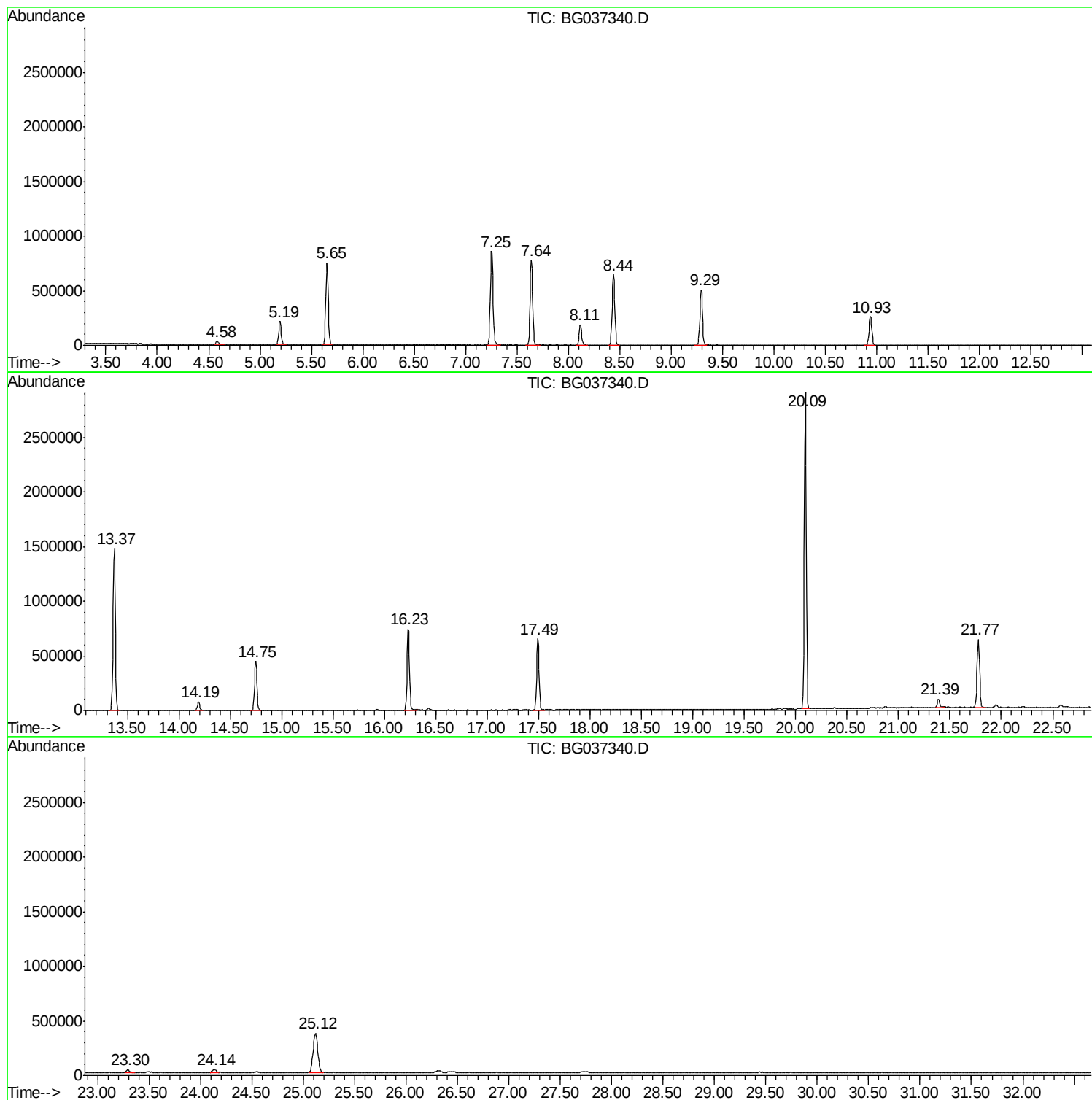
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.583	215	220	232	rVB	30872	49504	1.29%	0.260%
2	5.194	318	324	335	rBV	215062	344971	8.98%	1.811%
3	5.652	394	402	411	rBV	747304	1215258	31.65%	6.381%
4	7.250	666	674	689	rBV	857283	1551466	40.41%	8.147%
5	7.638	731	740	754	rBV	776932	1351040	35.19%	7.094%
6	8.114	814	821	832	rVB	188380	327796	8.54%	1.721%
7	8.437	868	876	885	rVB	642996	1120862	29.19%	5.886%
8	9.289	1010	1021	1030	rBV	504271	913849	23.80%	4.799%
9	10.934	1291	1301	1309	rBV	261585	483017	12.58%	2.536%
10	13.372	1707	1716	1724	rBV	1484075	2383346	62.07%	12.515%
11	14.189	1849	1855	1862	rBV	77148	118525	3.09%	0.622%
12	14.747	1941	1950	1958	rBV2	450236	733732	19.11%	3.853%
13	16.228	2196	2202	2217	rBV	741874	1168600	30.44%	6.136%
14	17.491	2410	2417	2428	rBV2	653188	1006086	26.20%	5.283%
15	20.094	2854	2860	2867	rBV	2901272	3839477	100.00%	20.161%
16	21.387	3075	3080	3090	rBV2	81240	148074	3.86%	0.778%
17	21.774	3140	3146	3157	rVB2	626661	1083220	28.21%	5.688%
18	23.296	3400	3405	3415	rVB4	24908	51253	1.33%	0.269%
19	24.136	3541	3548	3555	rBV3	30342	69813	1.82%	0.367%
20	25.123	3705	3716	3728	rVB2	358100	1084213	28.24%	5.693%

Sum of corrected areas: 19044102

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.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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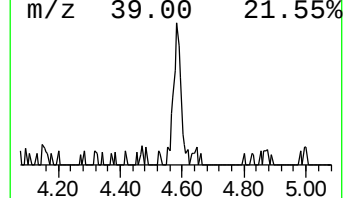
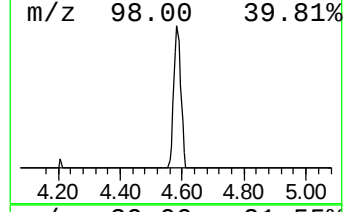
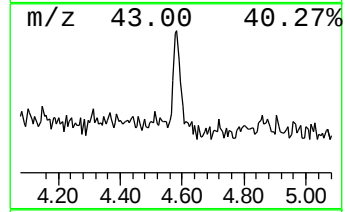
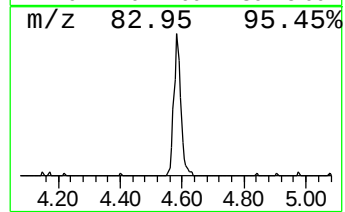
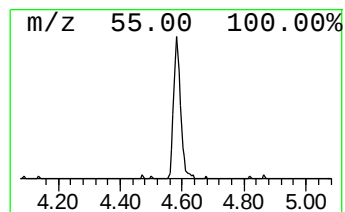
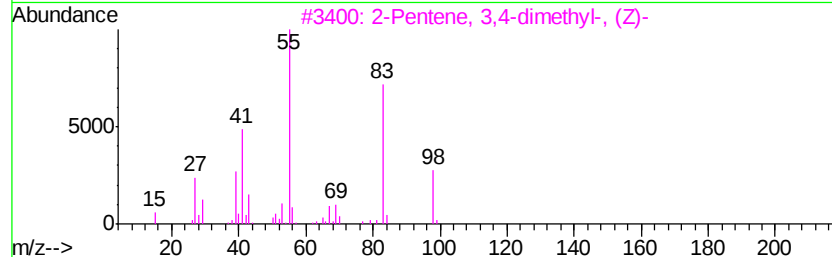
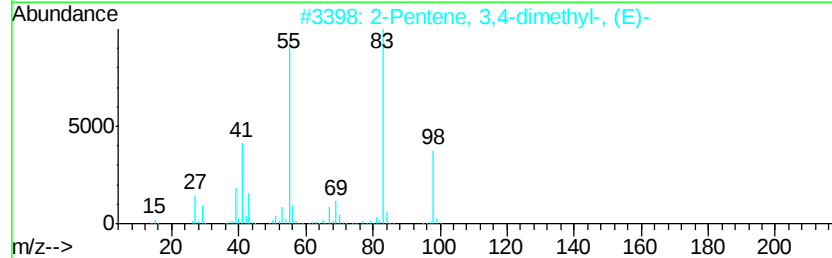
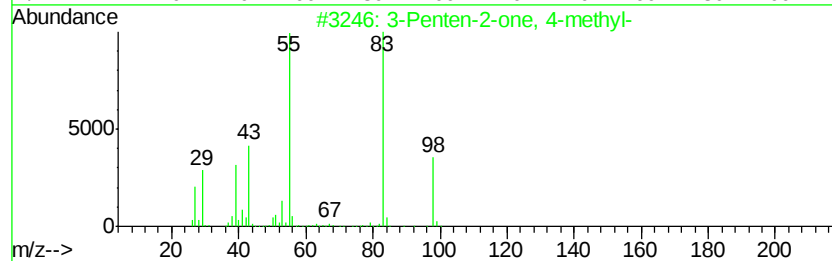
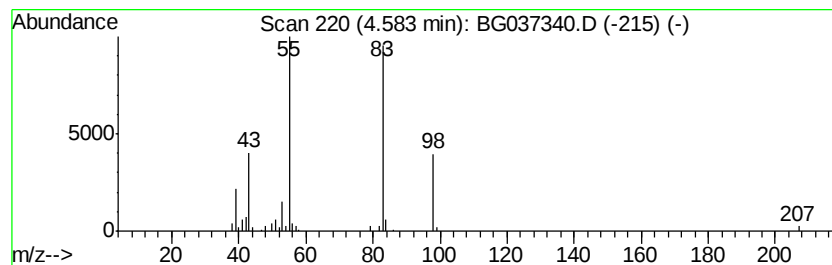
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG101118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.58	3.02 ng	49504	1,4-Dichlorobenzene-d4	8.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			Furan, 2-methoxy-	98	C5H6O2	025414-22-6	83
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	80



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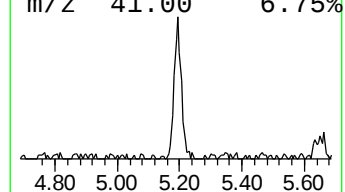
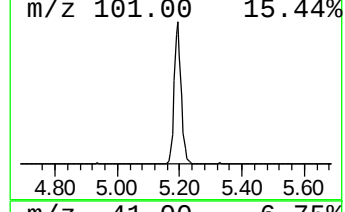
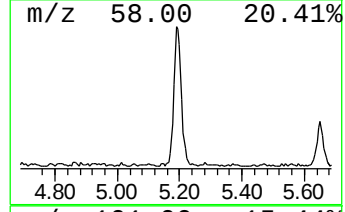
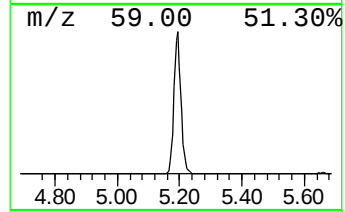
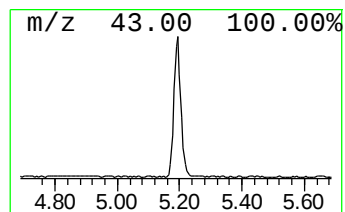
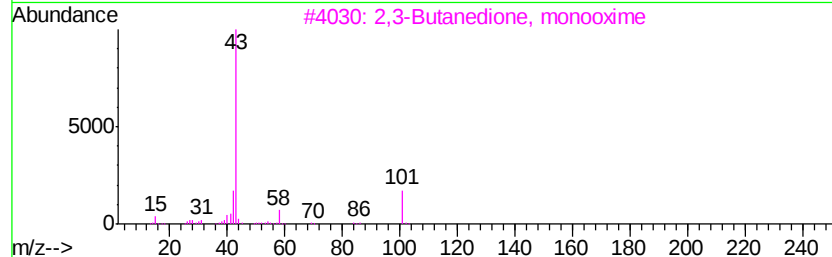
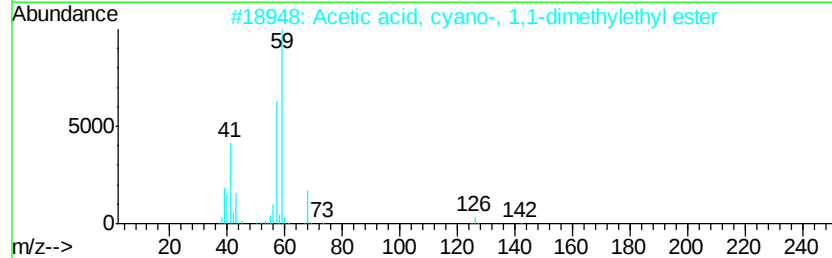
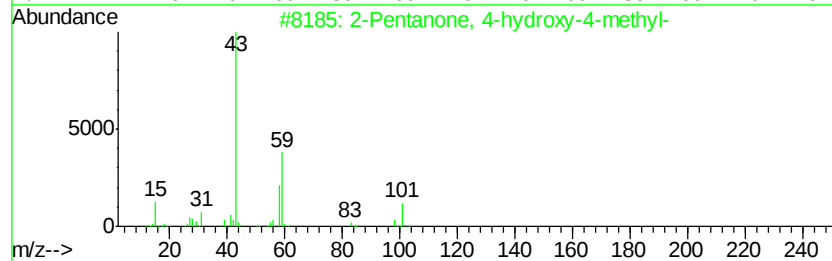
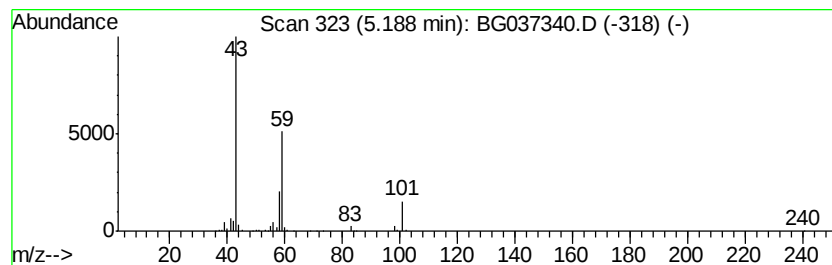
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	21.05 ng	344971	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
4		Thiocyanic acid, propyl ester	101	C4H7NS	004251-16-5	9
5		Acetone	58	C3H6O	000067-64-1	9



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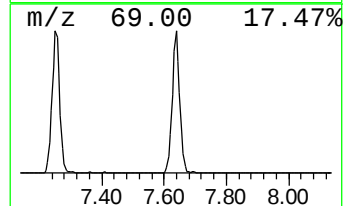
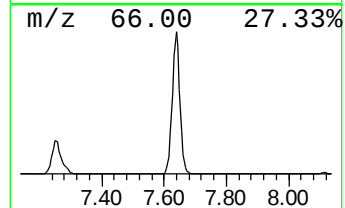
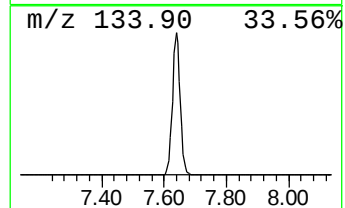
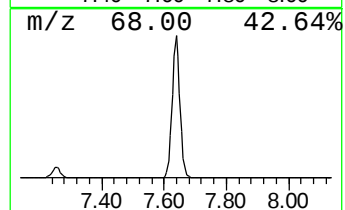
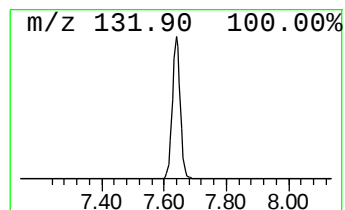
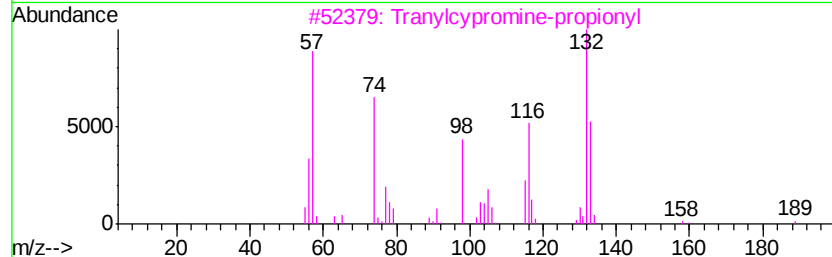
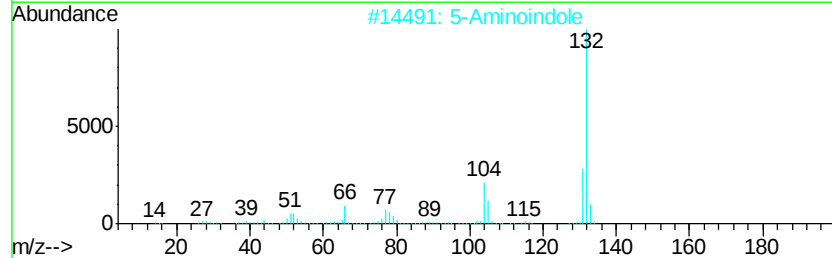
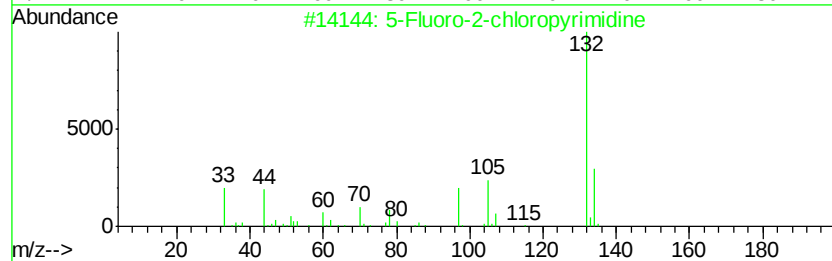
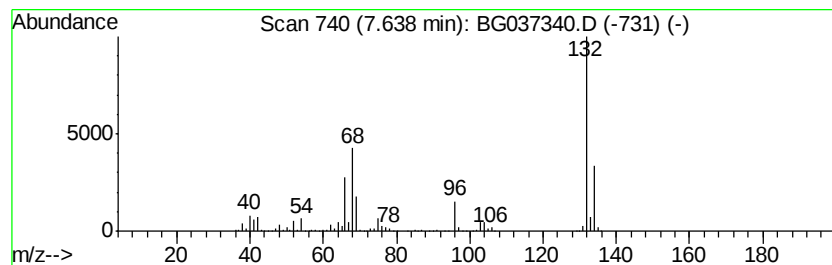
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Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	82.43 ng	1351040	1,4-Dichlorobenzene-d4	8.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
4			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5			1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	9



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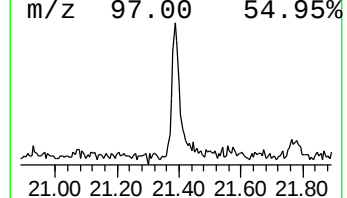
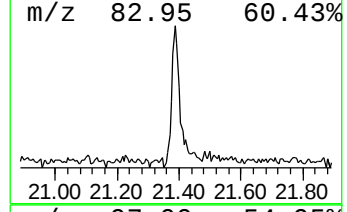
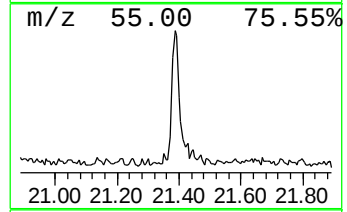
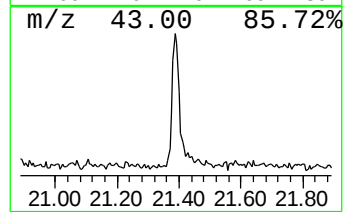
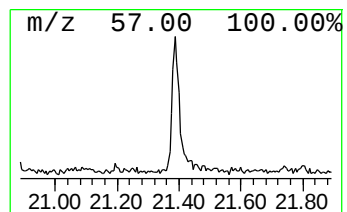
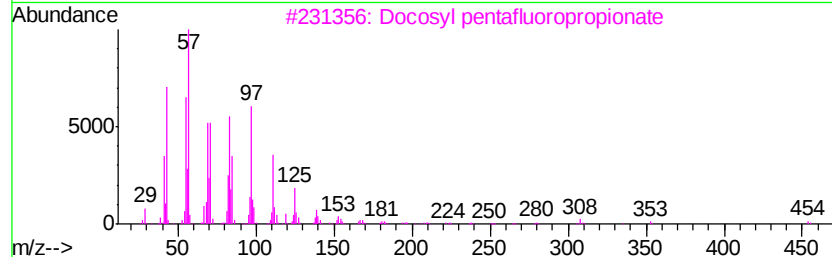
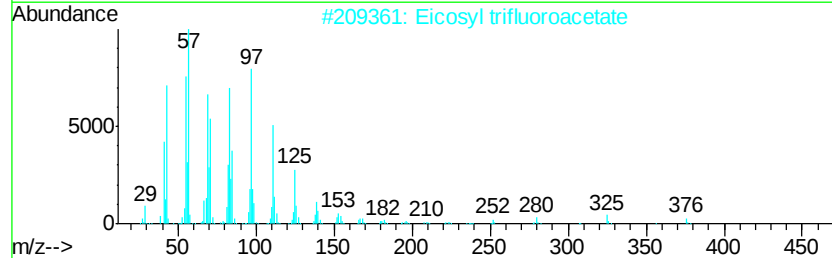
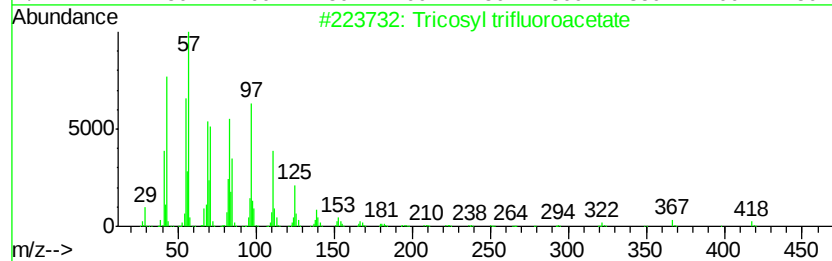
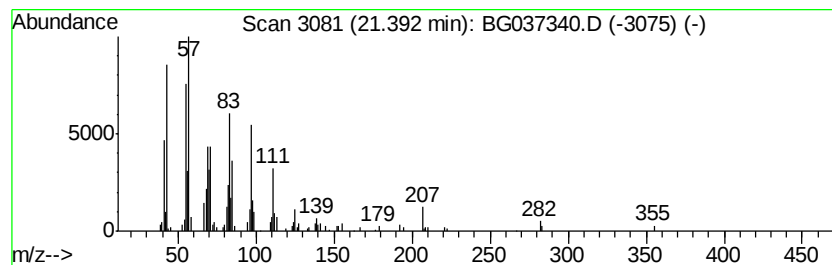
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Peak Number 5 Tricosyl trifluoroacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.39	2.73 ng	148074	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	87
2		Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	87
3		Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	87
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87
5		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.58	3.0	ng	49504	1	8.11	327796	20.0
2-Pentanone, 4-hy...	5.19	21.1	ng	344971	1	8.11	327796	20.0
unknown7.64	7.64	82.4	ng	1351040	1	8.11	327796	20.0
Tricosyl trifluor...	21.39	2.7	ng	148074	5	21.77	1083220	20.0