

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG010919\
 Data File : BG039033.D
 Acq On : 9 Jan 2019 23:05
 Operator : JU/SJ
 Sample : K1088-03
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CPSB-06(15-20)

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-BG010919.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	3.146	6	10	17	rVB2	11460	16422	1.06%	0.209%
2	3.704	101	105	117	rBV	11293	20306	1.32%	0.258%
3	5.108	340	344	351	rBV	16274	26081	1.69%	0.332%
4	5.578	416	424	436	rBV	293905	496960	32.21%	6.322%
5	7.188	690	698	711	rBV	337793	608348	39.44%	7.739%
6	7.558	753	761	773	rBV	314113	547927	35.52%	6.970%
7	8.029	835	841	852	rBV	67991	112106	7.27%	1.426%
8	8.352	889	896	904	rVB	221051	392631	25.45%	4.995%
9	9.210	1033	1042	1059	rBV	182299	348599	22.60%	4.435%
10	10.849	1314	1321	1328	rBV	92146	163241	10.58%	2.077%
11	13.287	1729	1736	1747	rBV	534126	839393	54.41%	10.678%
12	14.116	1871	1877	1884	rVB	74464	111122	7.20%	1.414%
13	14.674	1965	1972	1984	rVB2	161844	273830	17.75%	3.483%
14	16.160	2219	2225	2244	rBV	552278	884180	57.32%	11.248%
15	17.418	2433	2439	2450	rBV	255479	394207	25.55%	5.015%
16	20.020	2876	2882	2889	rBV	1155302	1542648	100.00%	19.624%
17	21.289	3093	3098	3109	rBV2	38061	72303	4.69%	0.920%
18	21.695	3161	3167	3175	rVB2	276434	465718	30.19%	5.924%
19	23.134	3407	3412	3418	rVB6	11719	22540	1.46%	0.287%
20	23.328	3438	3445	3453	rBV3	9076	18721	1.21%	0.238%
21	23.939	3541	3549	3557	rBV5	10242	23783	1.54%	0.303%
22	24.891	3704	3711	3716	rBV4	8556	21399	1.39%	0.272%
23	24.979	3716	3726	3741	rVB2	161880	458422	29.72%	5.832%

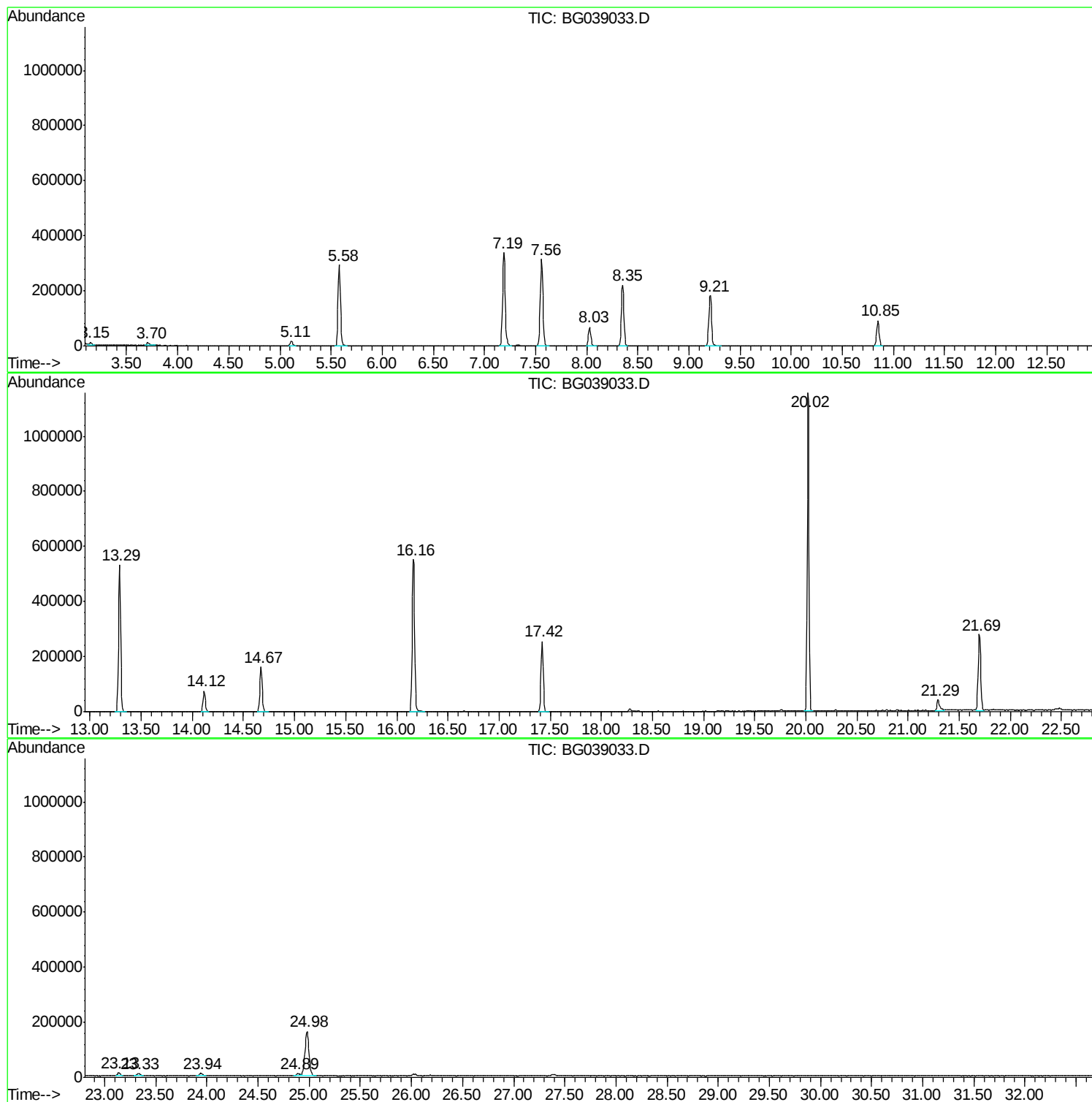
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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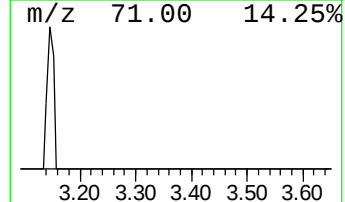
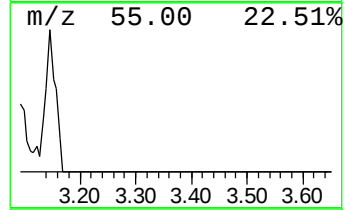
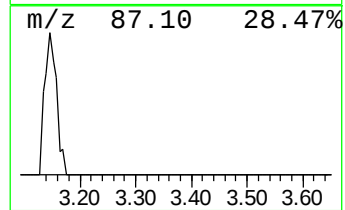
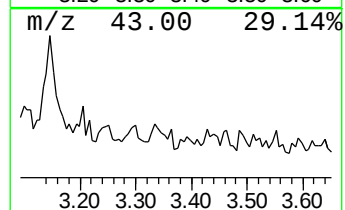
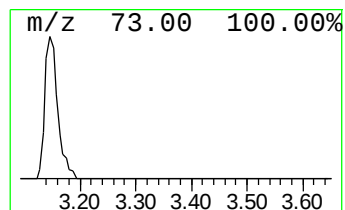
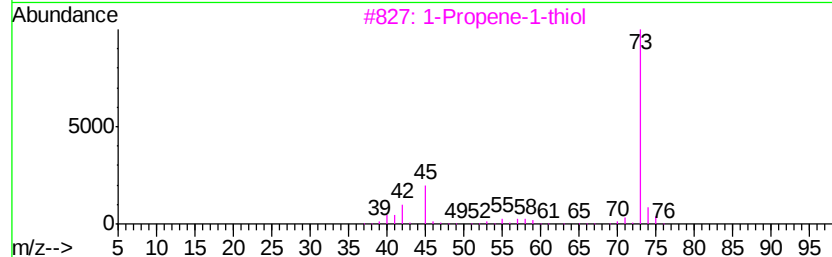
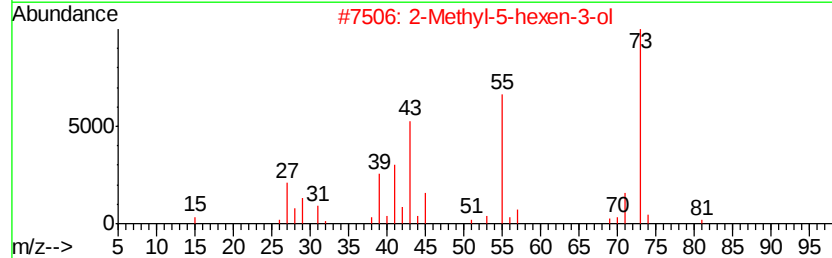
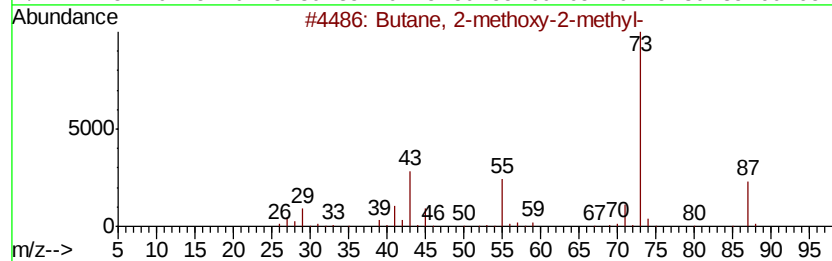
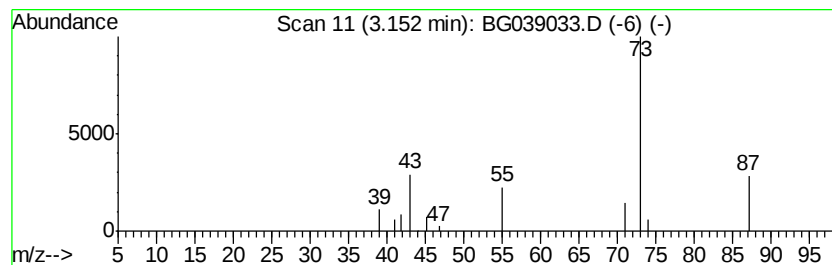
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG010919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.15	2.93 ng	16422	1,4-Dichlorobenzene-d4	8.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
3			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
4			1,3-Dioxolane, 2-(dichloromethyl)-	156	C4H6Cl2O2	002612-35-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5



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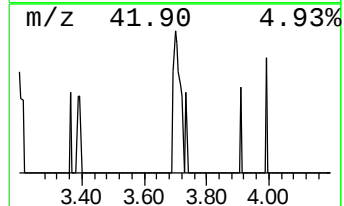
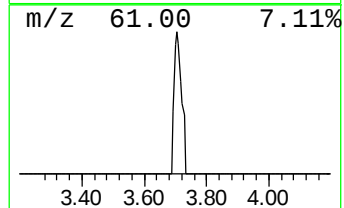
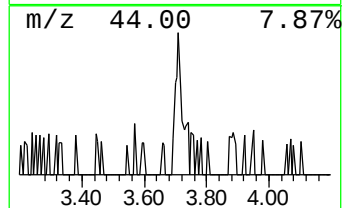
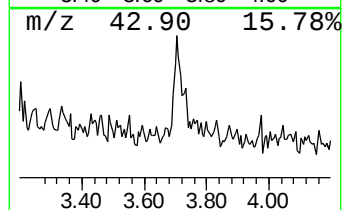
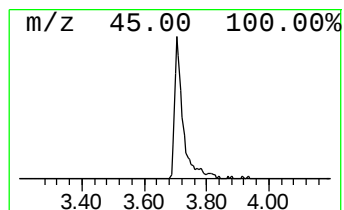
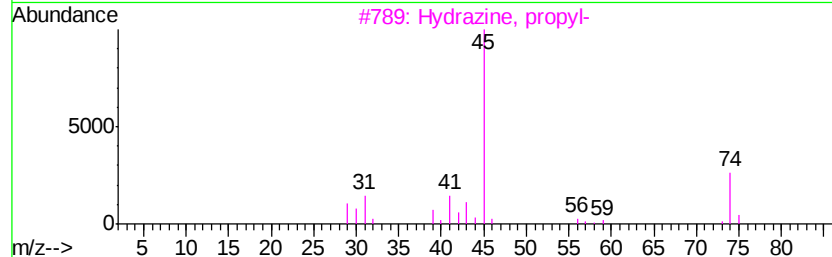
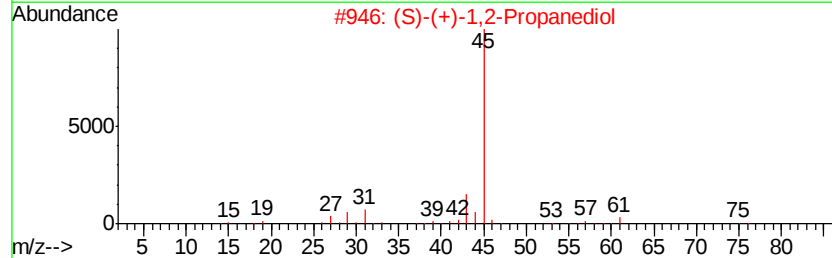
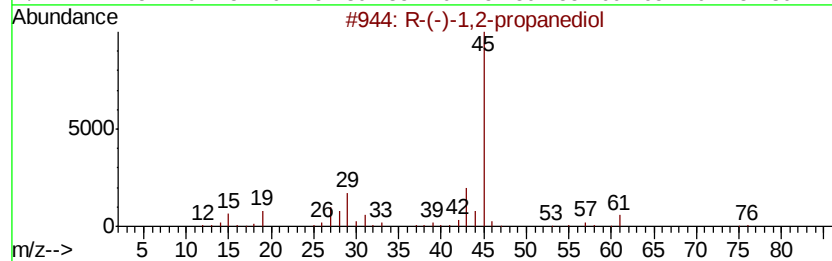
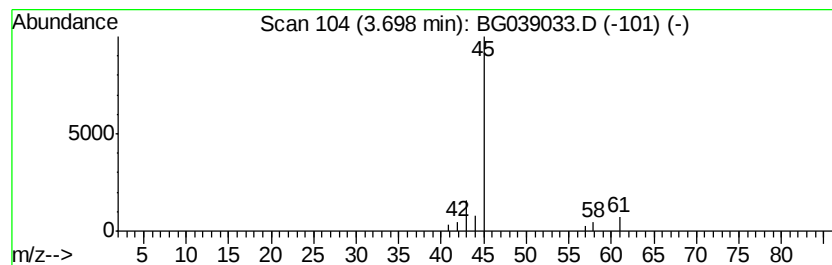
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Peak Number 2 R-(-)-1,2-propanediol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.70	3.62 ng	20306	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	64
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		Hydrazine, propyl-	74	C3H10N2	005039-61-2	9
4		Propylene Glycol	76	C3H8O2	000057-55-6	9
5		Isopropyl Alcohol	60	C3H8O	000067-63-0	9



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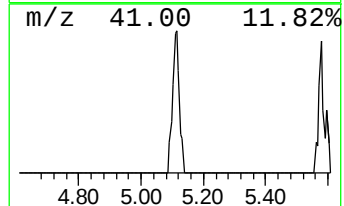
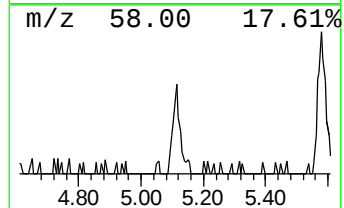
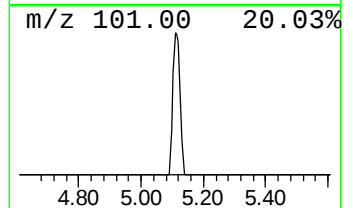
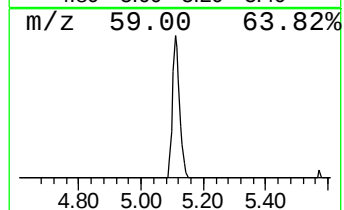
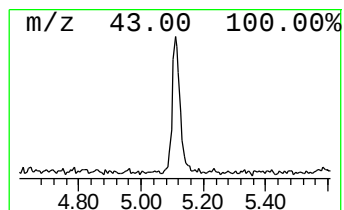
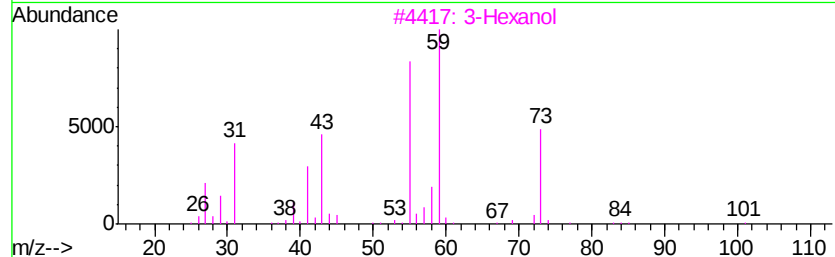
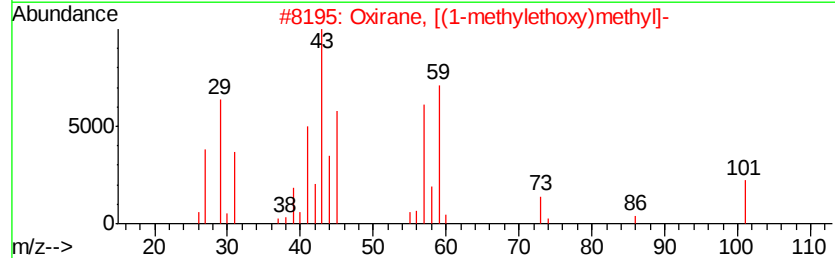
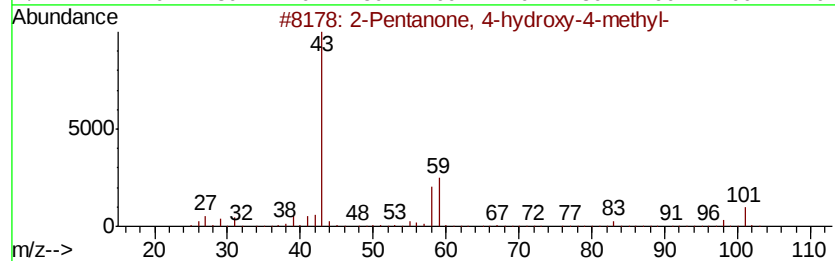
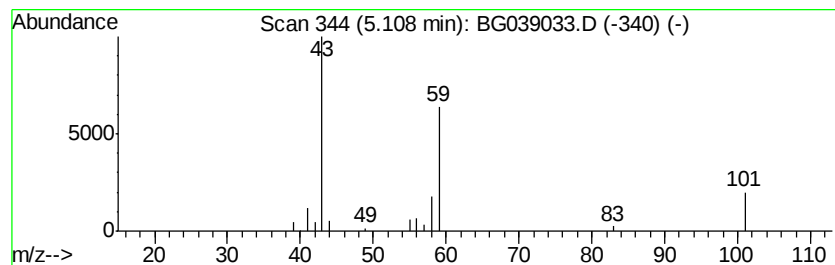
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	4.65 ng	26081	1,4-Dichlorobenzene-d4	8.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
3			3-Hexanol	102	C6H14O	000623-37-0	9
4			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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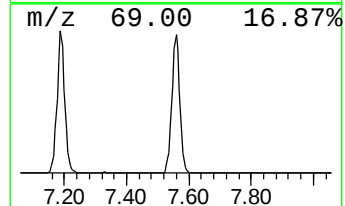
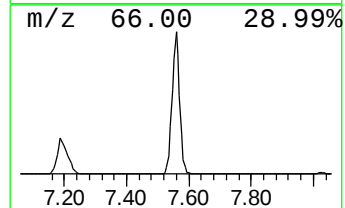
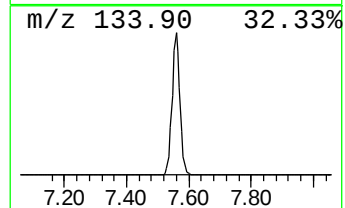
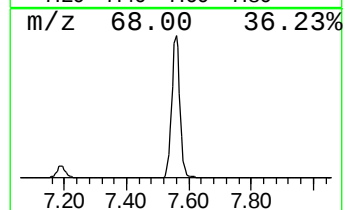
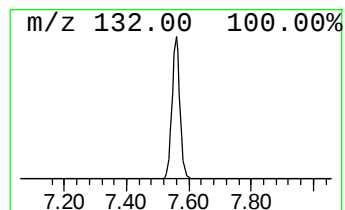
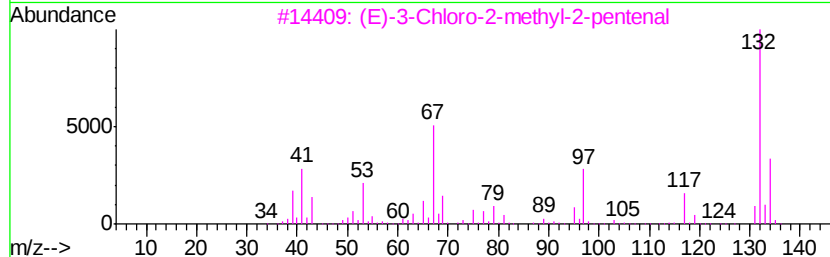
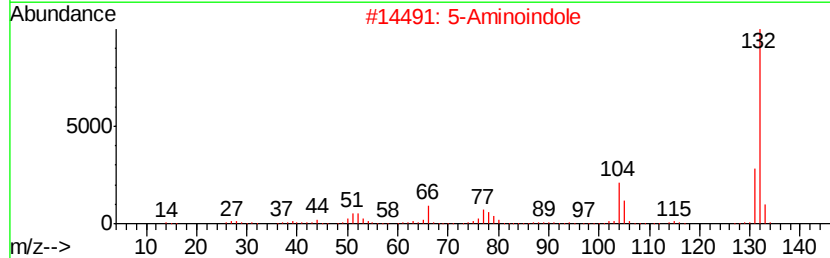
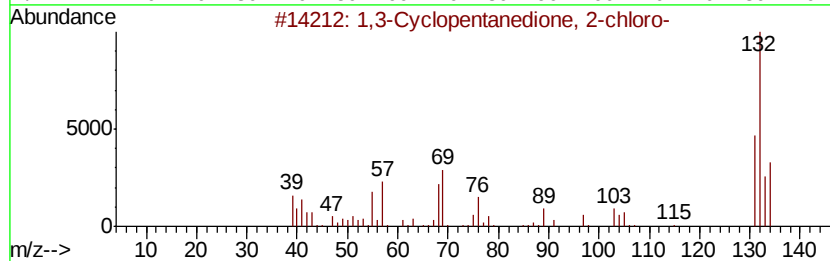
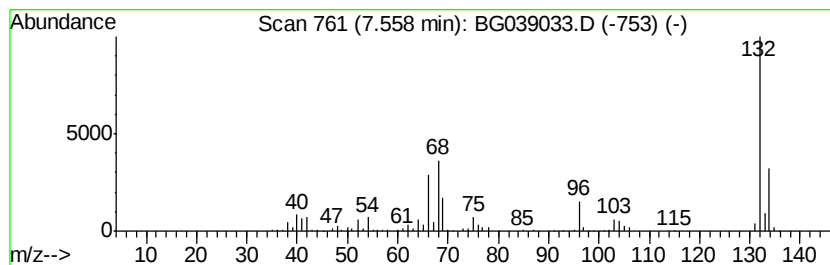
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Peak Number 4 unknown7.56 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.56	97.75 ng	547927	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	32
2		5-Aminoindole	132	C8H8N2	005192-03-0	27
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
5		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	12



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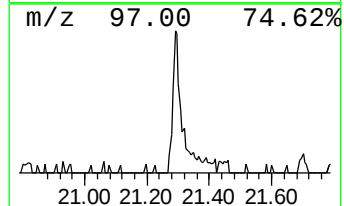
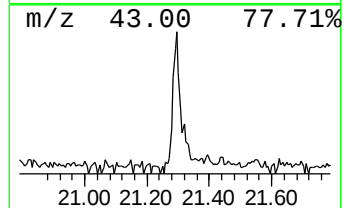
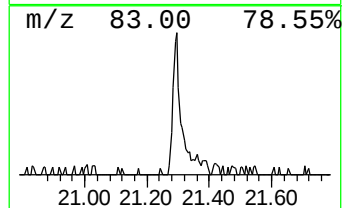
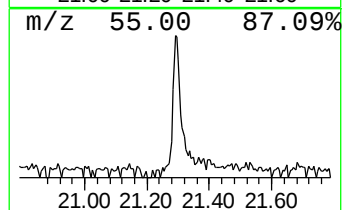
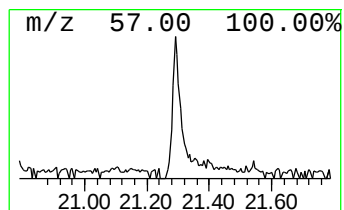
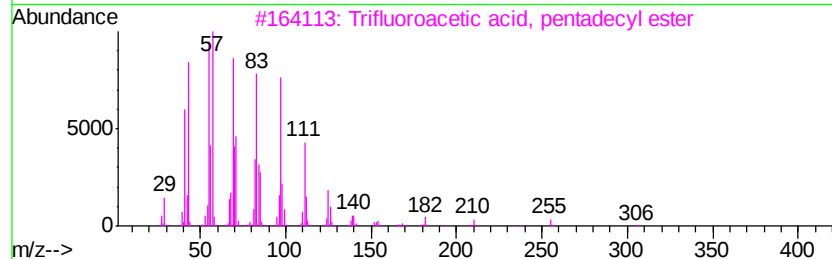
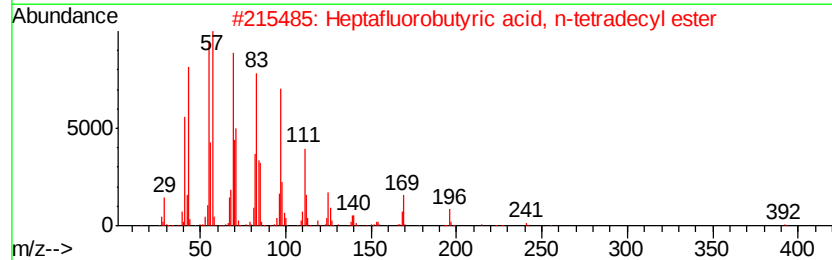
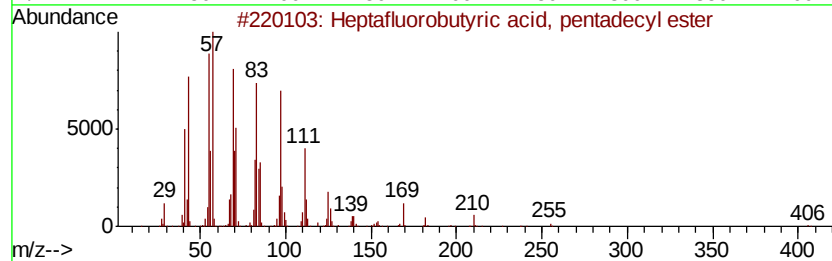
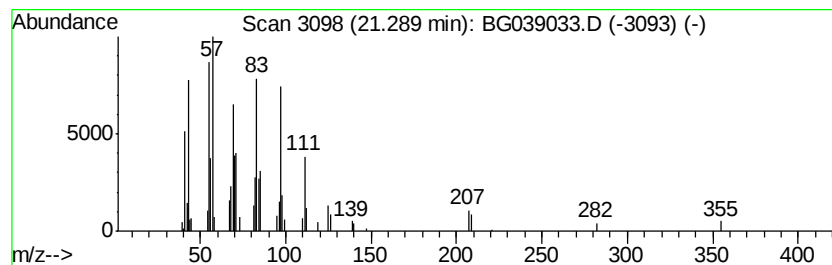
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Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.29	3.11 ng	72303	Chrysene-d12	21.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4		2-Chloropropionic acid, pentade...	318	C18H35ClO2	1000292-44-1	94
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.15	2.9	ng	16422	1	8.03	112106	20.0
R-(-)-1,2-propane...	3.70	3.6	ng	20306	1	8.03	112106	20.0
2-Pentanone, 4-hy...	5.11	4.7	ng	26081	1	8.03	112106	20.0
unknown7.56	7.56	97.8	ng	547927	1	8.03	112106	20.0
Heptafluorobutyri...	21.29	3.1	ng	72303	5	21.69	465718	20.0