

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG102618\
 Data File : BG037584.D
 Acq On : 26 Oct 2018 17:11
 Operator : JU/SJ
 Sample : J5649-11
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 DL-04B

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-BG101818.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	3.763	77	81	92	rBV	39998	69906	1.51%	0.264%
2	5.185	317	323	331	rBV	61563	105961	2.28%	0.400%
3	5.643	394	401	414	rVB	1166257	1944125	41.89%	7.340%
4	7.247	665	674	686	rBV	1272825	2465846	53.14%	9.310%
5	7.629	730	739	751	rBV	1174130	2093067	45.10%	7.903%
6	8.105	813	820	833	rBV	206761	373348	8.05%	1.410%
7	8.428	866	875	884	rVB	849589	1535948	33.10%	5.799%
8	9.280	1009	1020	1031	rBV	770105	1429723	30.81%	5.398%
9	10.925	1291	1300	1310	rVB	302805	569913	12.28%	2.152%
10	13.358	1706	1714	1725	rBV	2146344	3427008	73.85%	12.939%
11	14.180	1847	1854	1861	rBV	311673	464300	10.01%	1.753%
12	14.739	1941	1949	1957	rBV2	499484	860816	18.55%	3.250%
13	16.219	2194	2201	2219	rBV	1606159	2604879	56.13%	9.835%
14	17.482	2409	2416	2424	rBV2	711700	1102188	23.75%	4.162%
15	18.340	2555	2562	2575	rBV	131161	225105	4.85%	0.850%
16	19.603	2773	2777	2783	rBV3	47634	76634	1.65%	0.289%
17	20.079	2852	2858	2867	rBV	3255994	4640629	100.00%	17.522%
18	21.372	3073	3078	3092	rBV2	86186	194658	4.19%	0.735%
19	21.766	3138	3145	3158	rVB	645684	1136401	24.49%	4.291%
20	24.081	3533	3539	3552	rBV5	23436	62306	1.34%	0.235%
21	25.097	3699	3712	3728	rBV2	325239	1102436	23.76%	4.162%

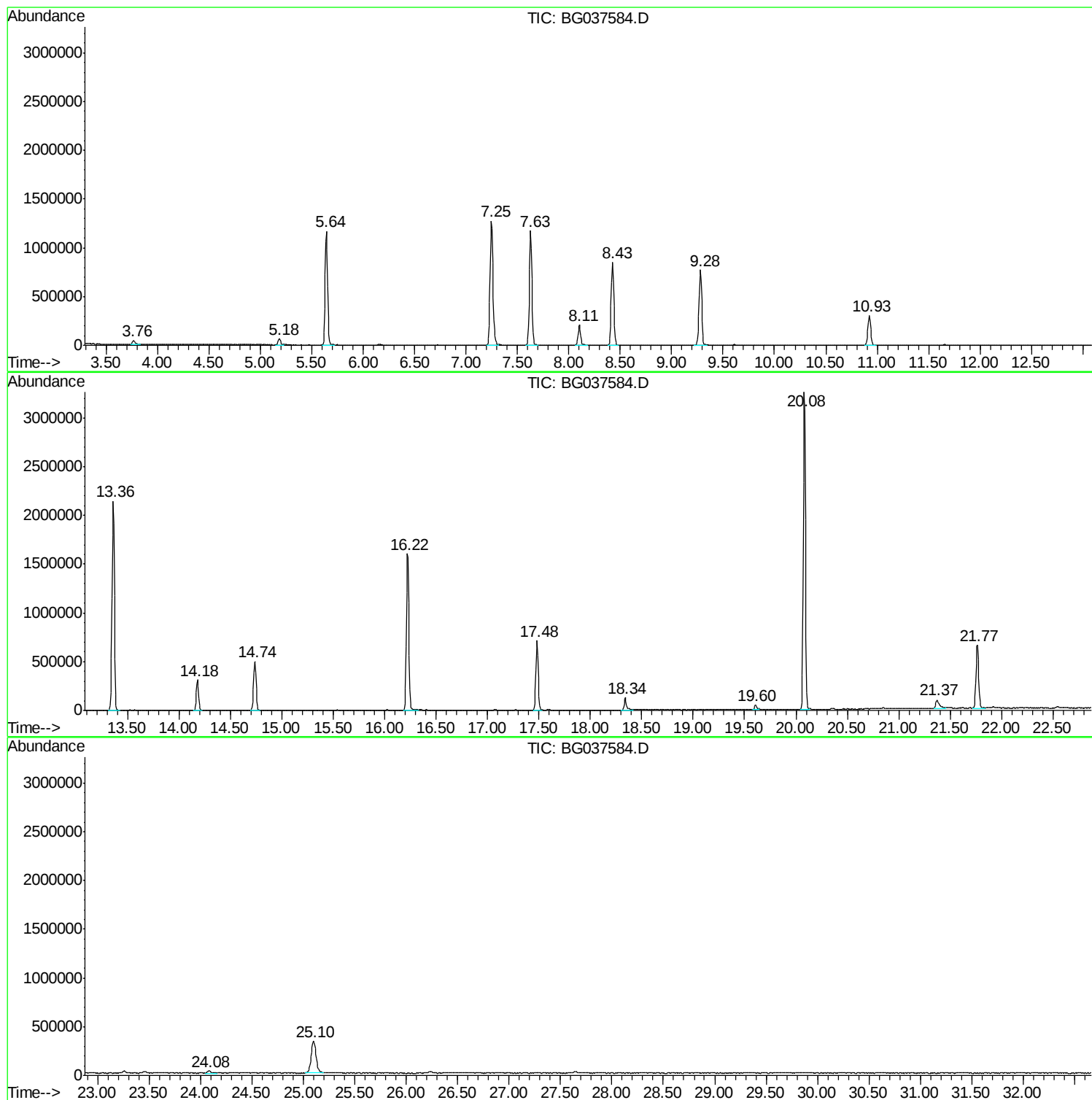
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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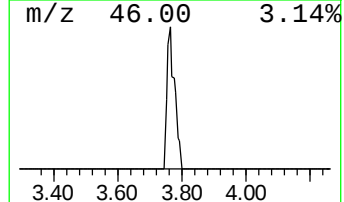
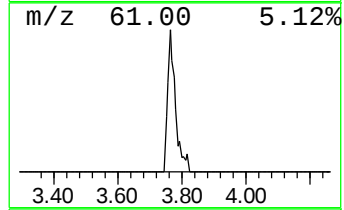
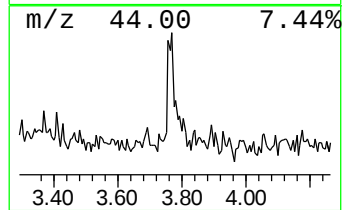
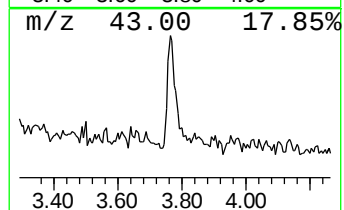
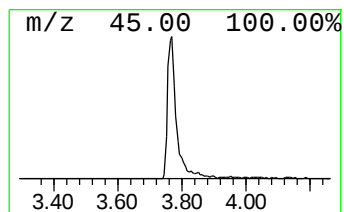
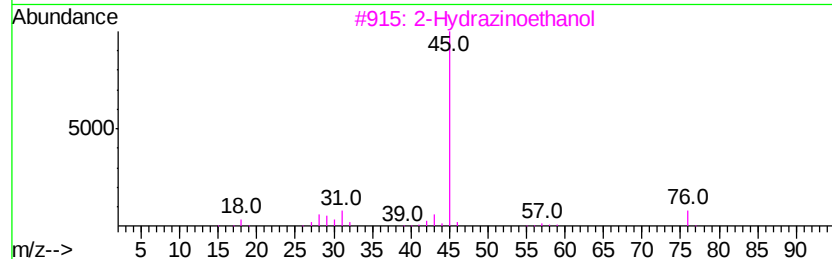
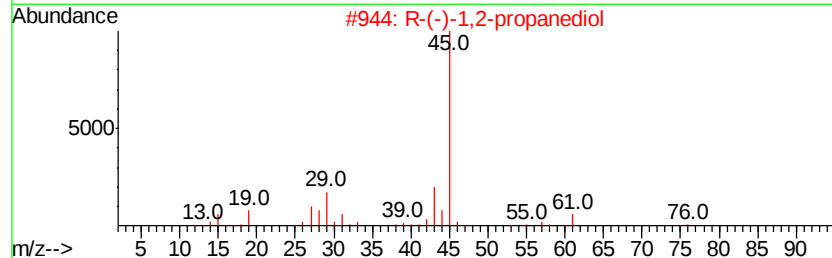
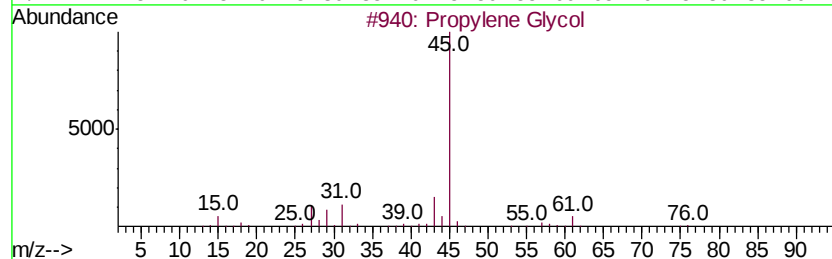
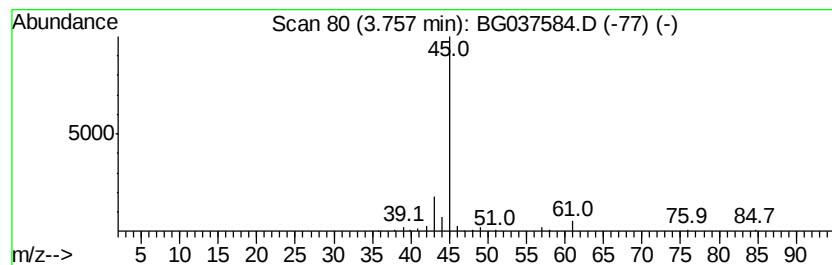
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG101818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.76 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.76	3.74 ng	69906	1,4-Dichlorobenzene-d4	8.11

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	43
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	2-Hydrazinoethanol	76	C2H8N2O	000109-84-2	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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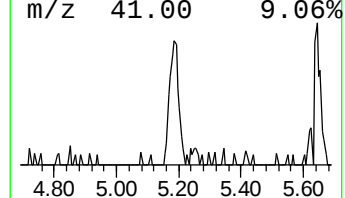
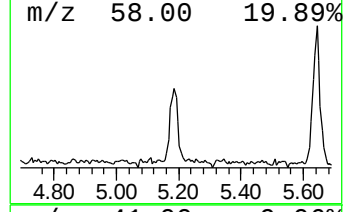
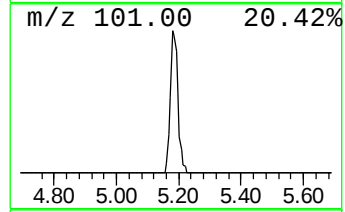
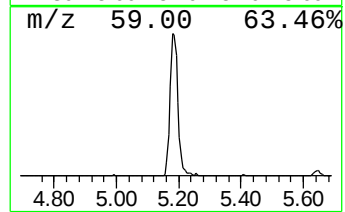
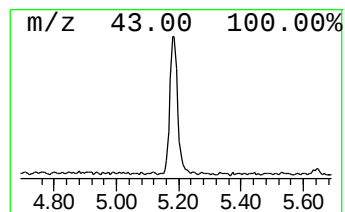
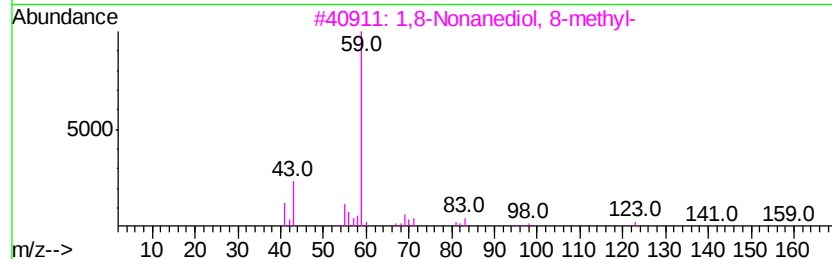
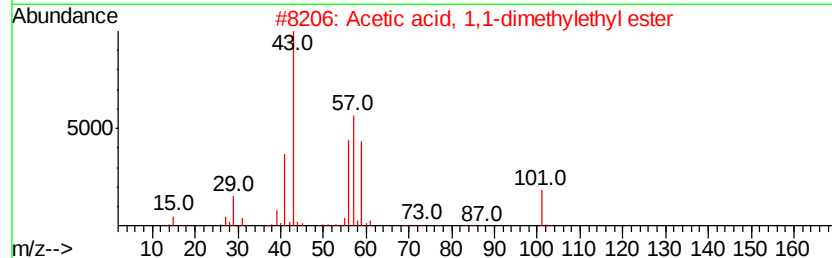
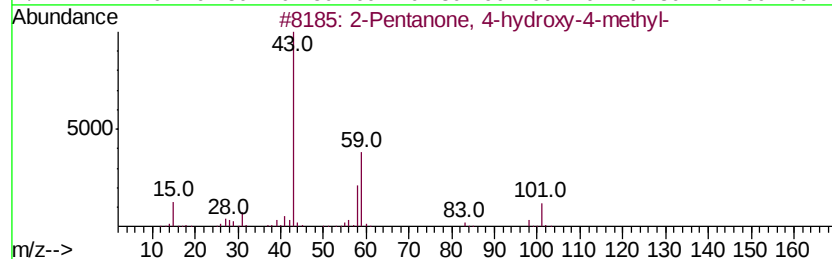
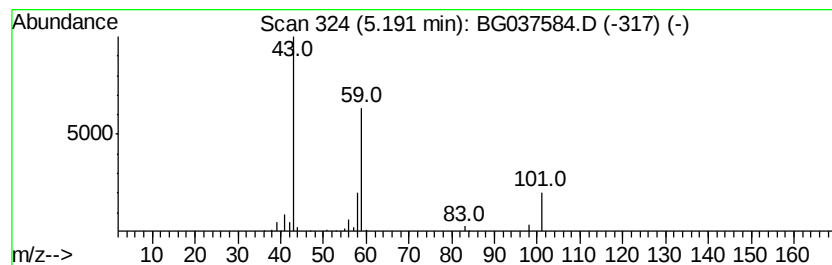
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	5.68 ng	105961	1,4-Dichlorobenzene-d4	8.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16



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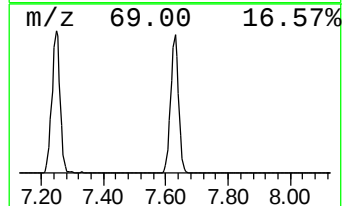
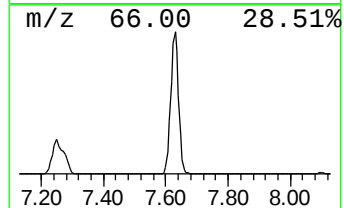
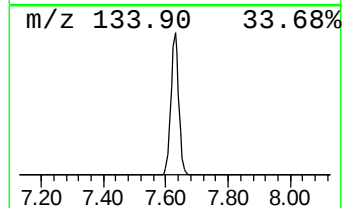
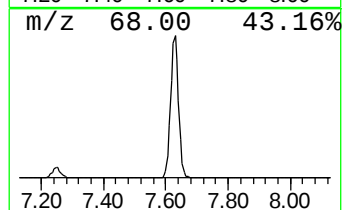
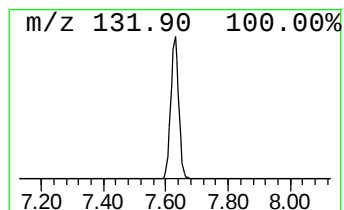
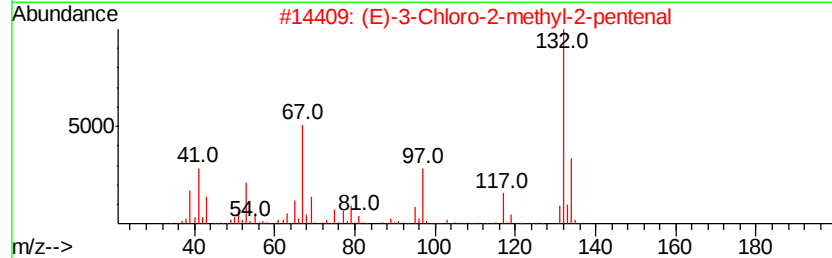
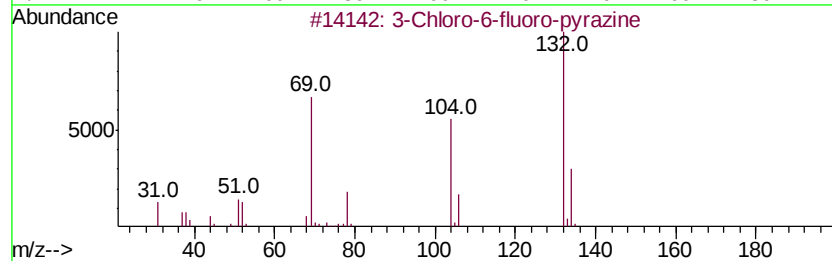
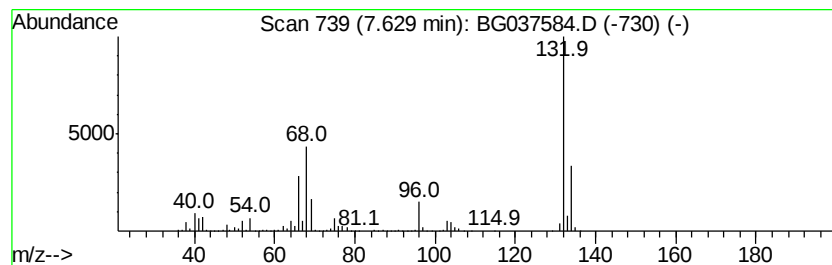
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Peak Number 3 unknown7.63 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	112.12 ng	2093070	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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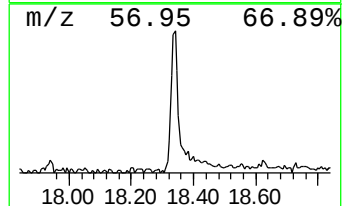
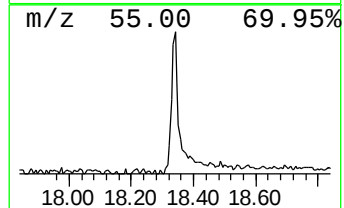
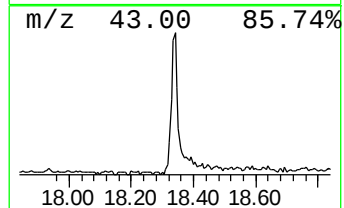
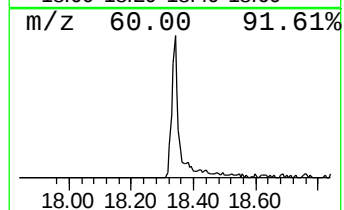
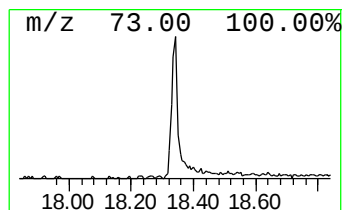
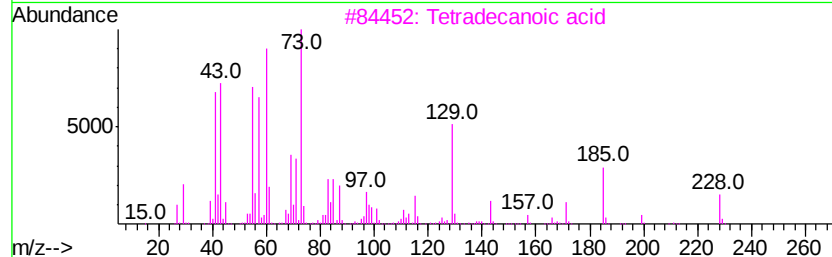
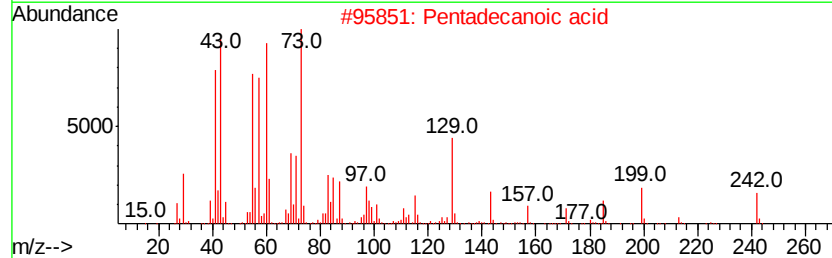
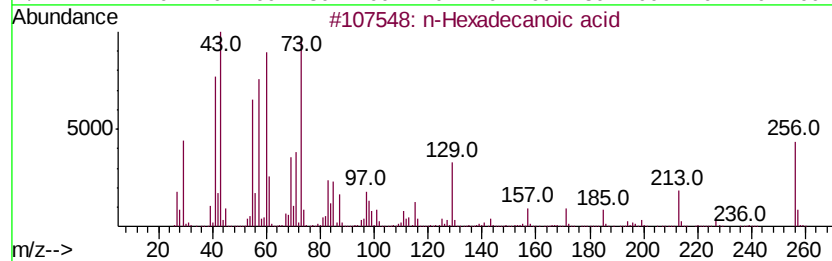
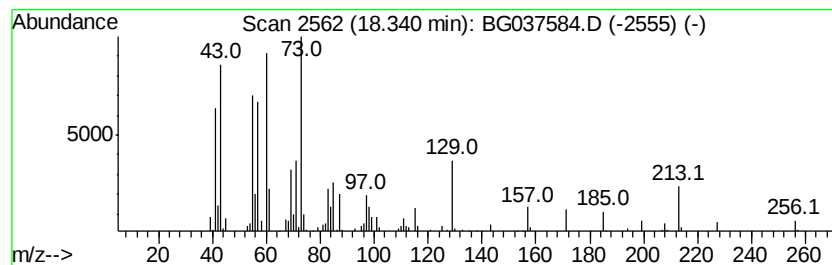
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.34	4.08 ng	225105	Phenanthrene-d10	17.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4		Tridecanoic acid	214	C13H26O2	000638-53-9	74
5		Undecanoic acid	186	C11H22O2	000112-37-8	59



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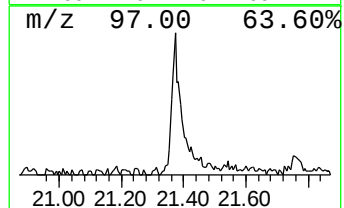
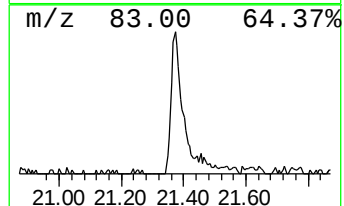
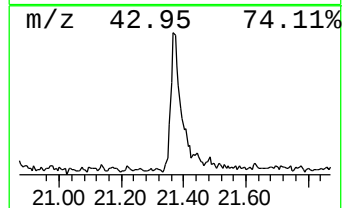
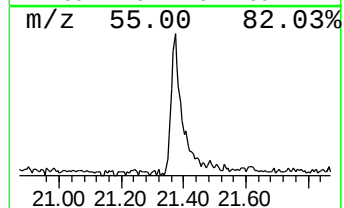
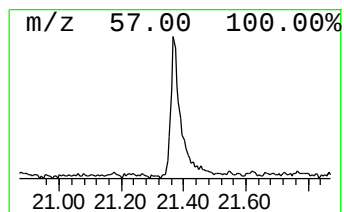
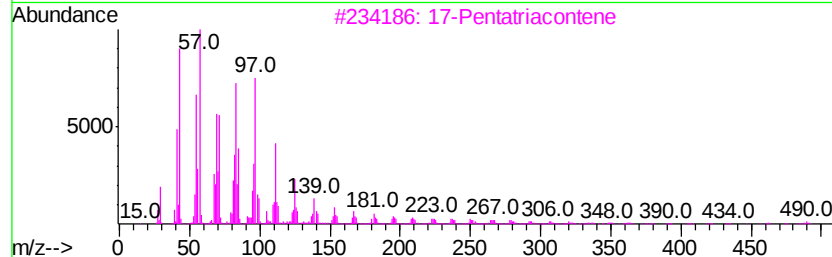
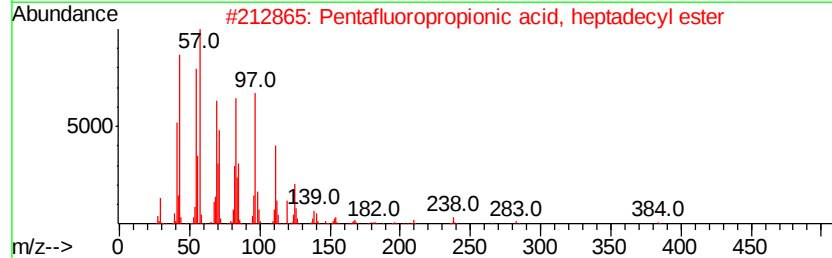
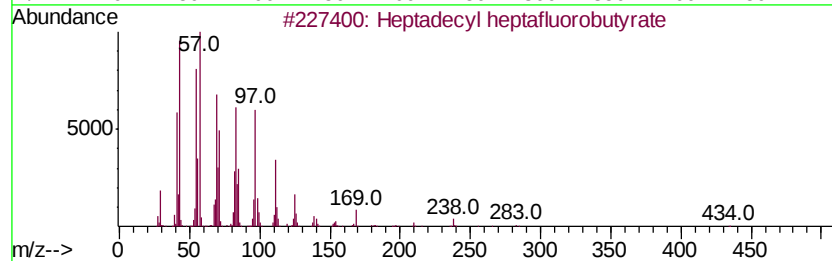
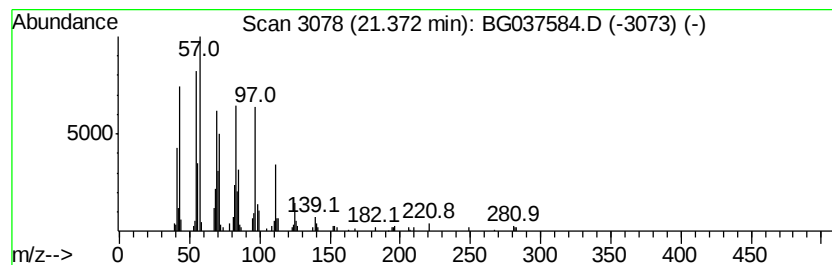
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Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.37	3.43 ng	194658	Chrysene-d12	21.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
3		17-Pentatriacontene	491	C35H70	006971-40-0	91
4		Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
5		Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.76	3.76	3.7	ng	69906	1	8.11	373348	20.0
2-Pentanone, 4-hy...	5.19	5.7	ng	105961	1	8.11	373348	20.0
unknown7.63	7.63	112.1	ng	2093070	1	8.11	373348	20.0
n-Hexadecanoic acid	18.34	4.1	ng	225105	4	17.48	1102190	20.0
Heptadecyl heptaf...	21.37	3.4	ng	194658	5	21.77	1136400	20.0