

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF052317\
 Data File : BF095363.D
 Acq On : 23 May 2017 21:33
 Operator : SJ/MA
 Sample : I3249-06
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-14COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF050217.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	5.131	540	543	559	rBV	108492	242504	7.20%	0.998%
2	5.719	639	643	668	rBV	1138198	2577369	76.51%	10.603%
3	7.301	908	912	928	rBV	1533612	2602012	77.24%	10.705%
4	7.419	928	932	945	rVB	1922785	3140141	93.22%	12.919%
5	7.754	985	989	1001	rVB	462054	574813	17.06%	2.365%
6	7.989	1024	1029	1049	rVB	1758394	2324400	69.00%	9.563%
7	8.654	1138	1142	1171	rBV	937040	1702669	50.54%	7.005%
8	9.777	1329	1333	1362	rBV	393839	791049	23.48%	3.254%
9	11.542	1628	1633	1651	rBV	2290406	3368659	100.00%	13.859%
10	12.060	1715	1721	1733	rBV	83564	127205	3.78%	0.523%
11	12.248	1749	1753	1769	rBV	189076	324777	9.64%	1.336%
12	12.607	1809	1814	1827	rBV2	527014	832156	24.70%	3.423%
13	13.436	1952	1955	1960	rVB2	33299	36077	1.07%	0.148%
14	13.901	2029	2034	2058	rBV	930928	1683901	49.99%	6.928%
15	14.212	2083	2087	2095	rBV	28239	40730	1.21%	0.168%
16	15.012	2219	2223	2246	rVB	376000	685485	20.35%	2.820%
17	15.965	2381	2385	2394	rBV3	49967	91832	2.73%	0.378%
18	17.330	2612	2617	2627	rBV	1754641	2186676	64.91%	8.996%
19	18.577	2823	2829	2844	rBV5	25872	96948	2.88%	0.399%
20	18.689	2844	2848	2864	rVV	245110	409505	12.16%	1.685%
21	19.147	2922	2926	2932	rBV	31220	36481	1.08%	0.150%
22	20.365	3129	3133	3142	rBV	259282	431805	12.82%	1.776%

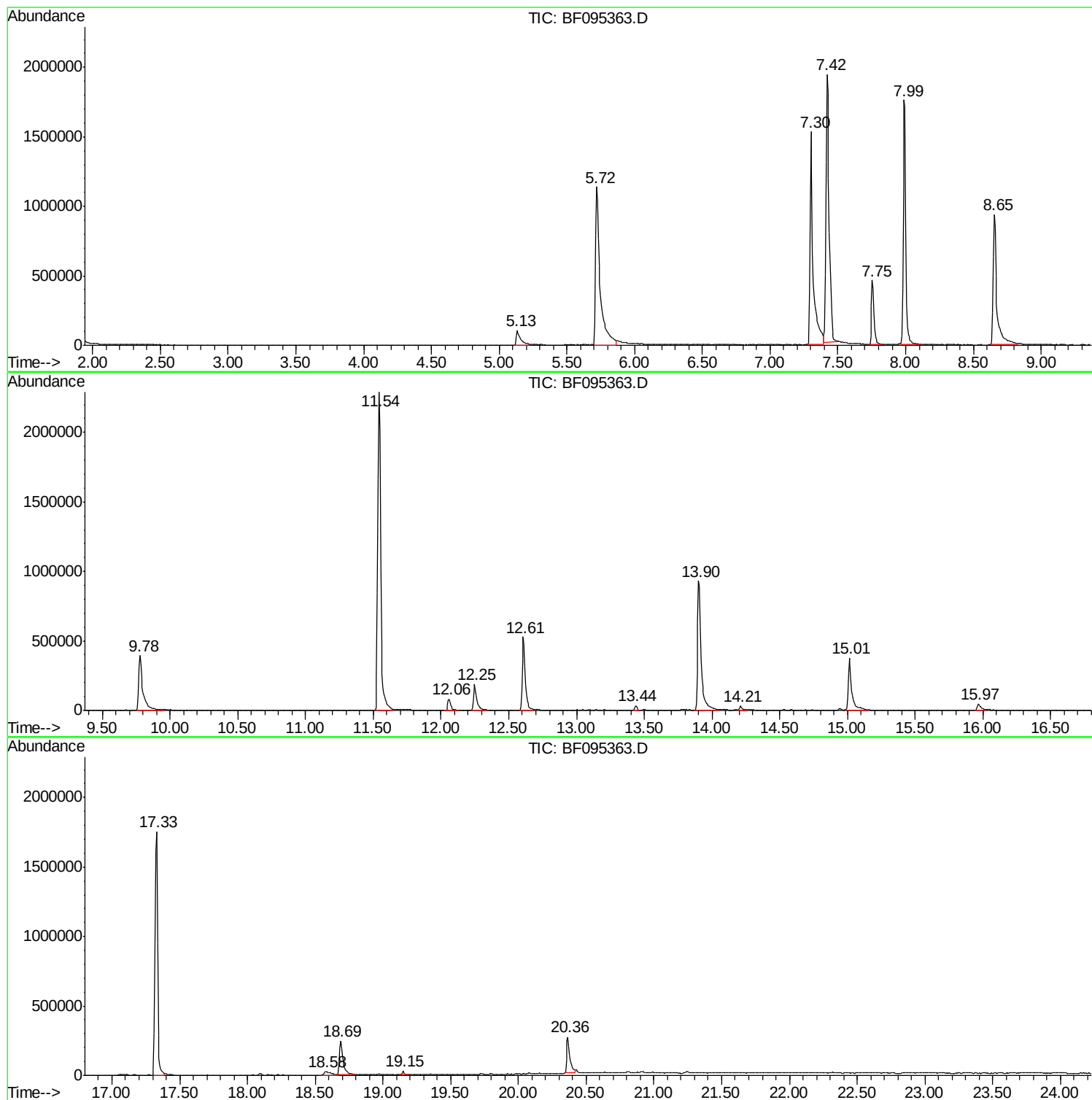
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050217.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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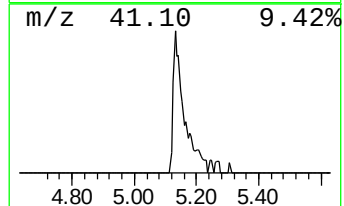
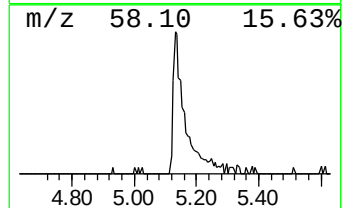
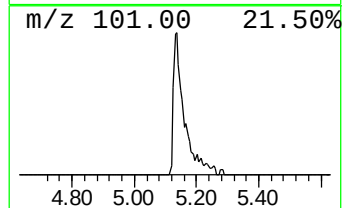
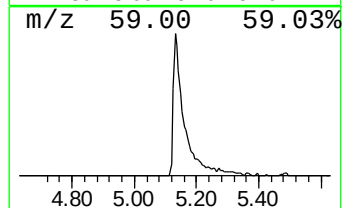
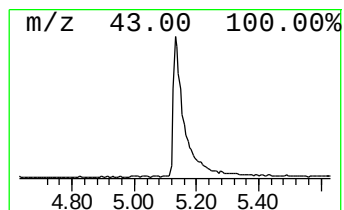
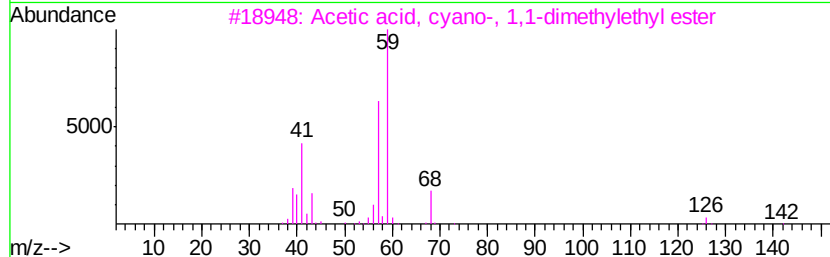
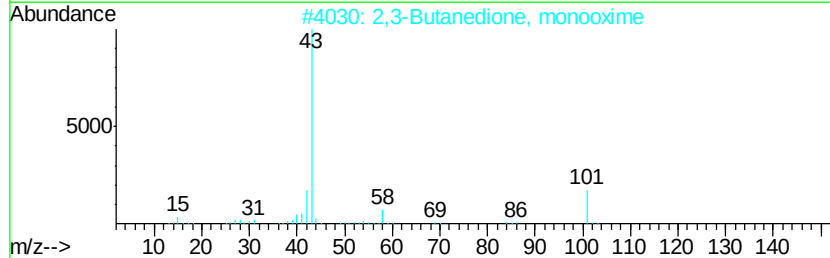
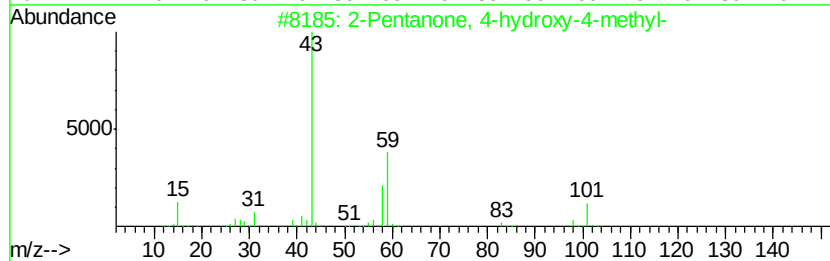
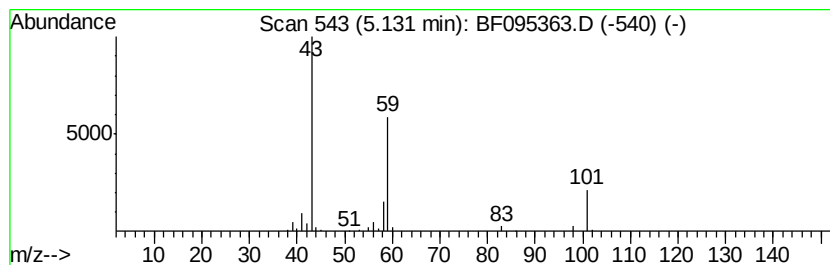
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	8.44 ng	242504	1,4-Dichlorobenzene-d4	7.75

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	32
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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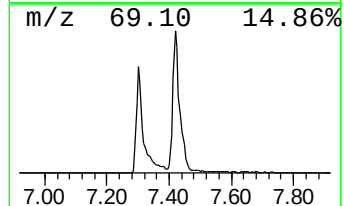
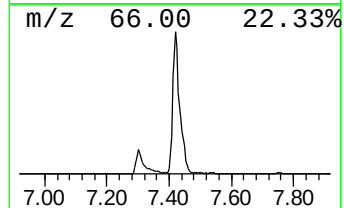
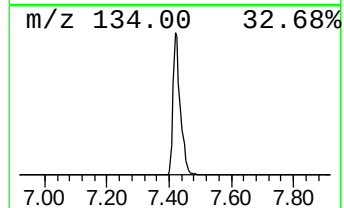
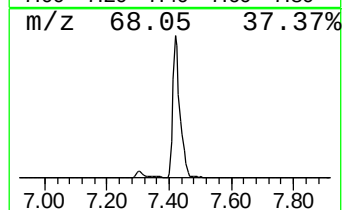
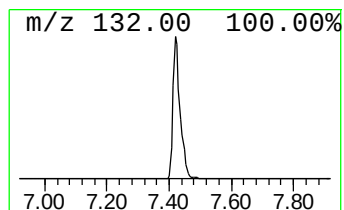
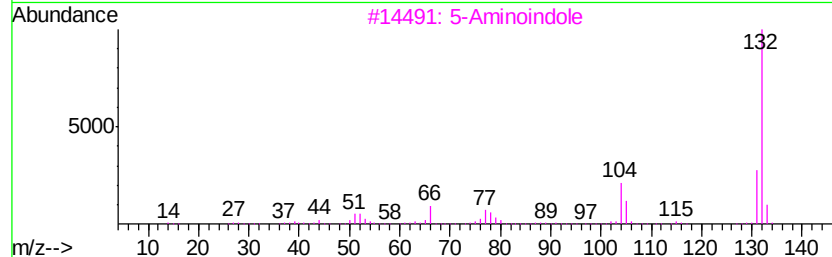
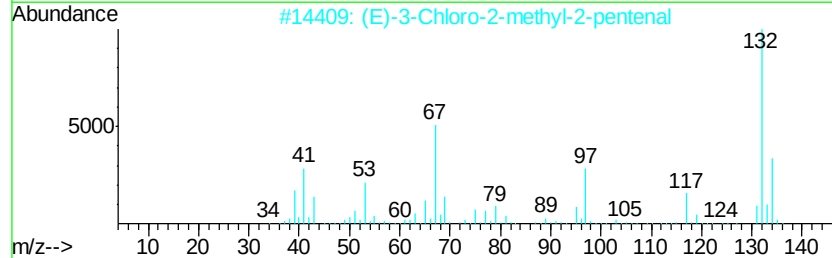
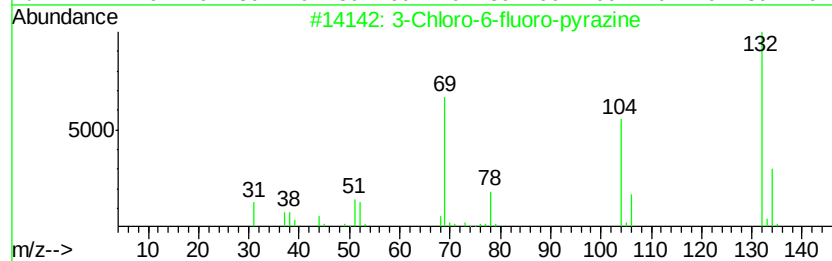
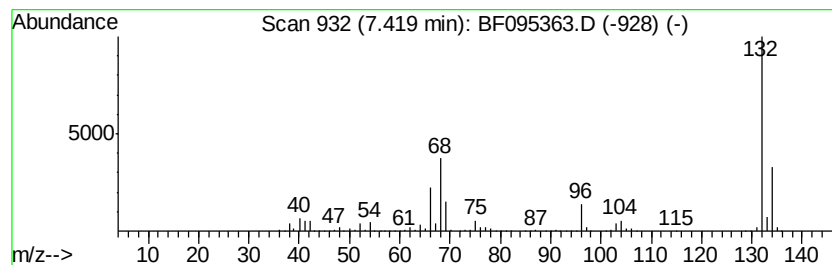
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Peak Number 2 unknown7.42 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.42	109.26 ng	3140140	1,4-Dichlorobenzene-d4	7.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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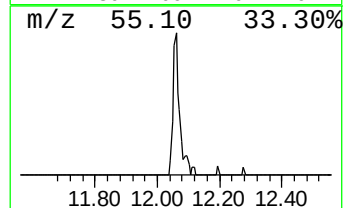
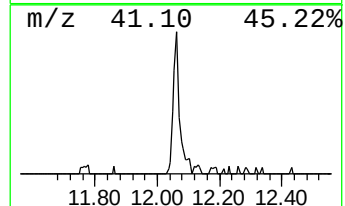
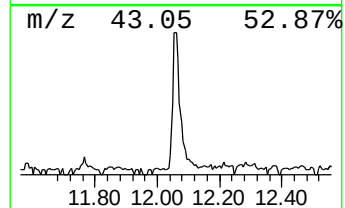
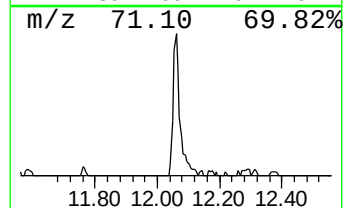
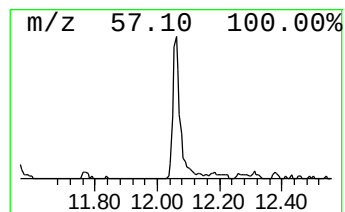
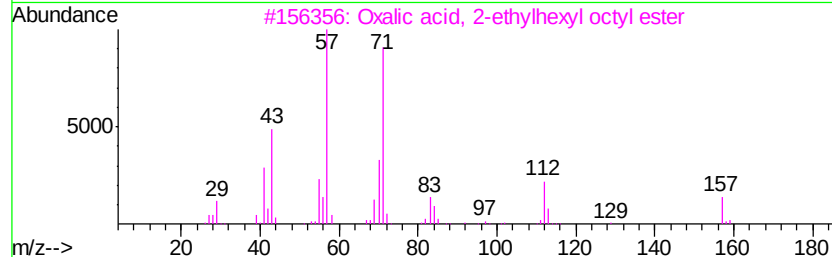
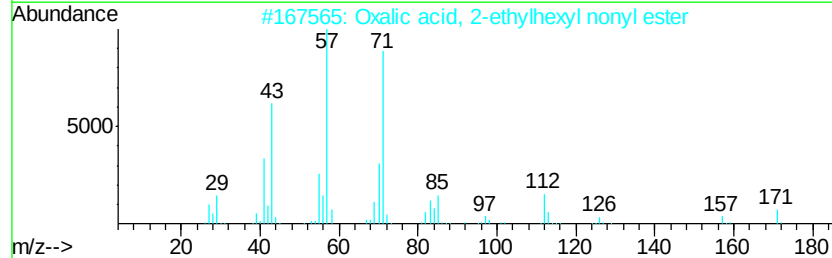
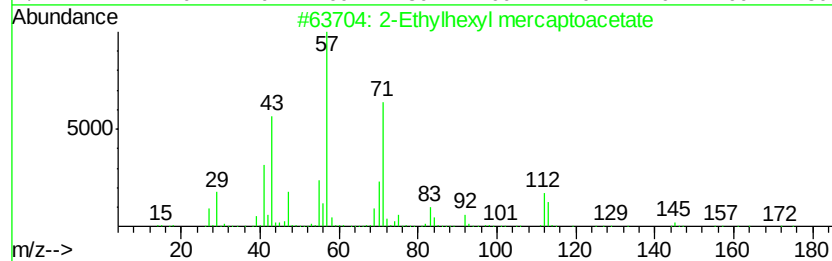
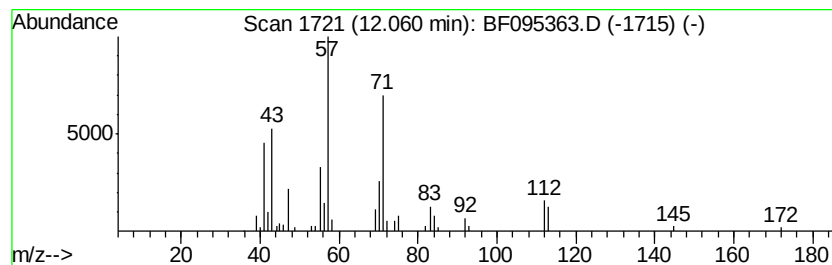
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Peak Number 4 2-Ethylhexyl mercaptoacetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.06	3.06 ng	127205	Acenaphthene-d10	12.61	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	91
2	Oxalic acid, 2-ethylhexyl nonyl ...	328	C19H36O4	1000309-39-2	58
3	Oxalic acid, 2-ethylhexyl octyl ...	314	C18H34O4	1000309-39-1	58
4	Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1000309-38-5	58
5	Oxalic acid, butyl 2-ethylhexyl ...	258	C14H26O4	1000309-38-6	53



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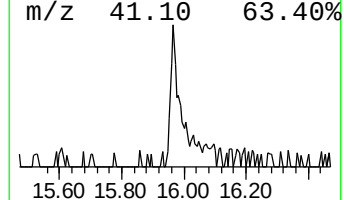
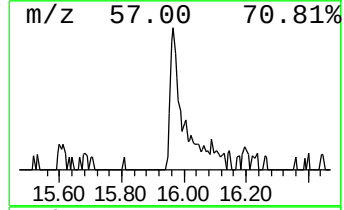
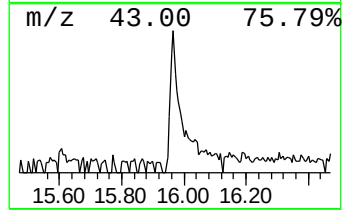
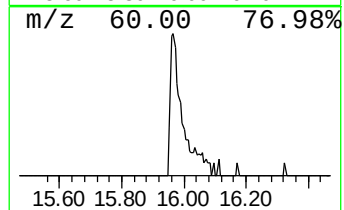
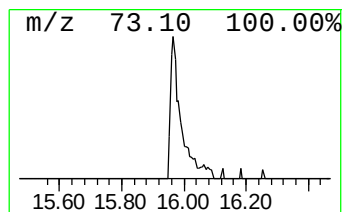
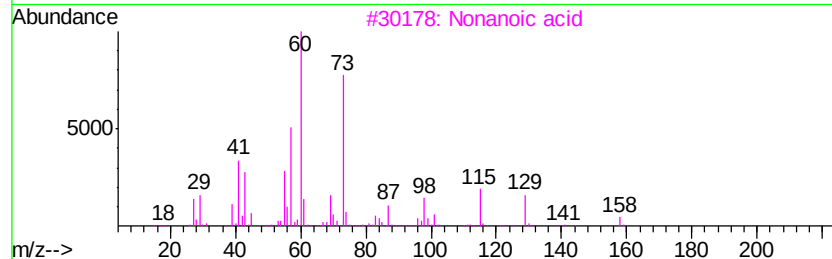
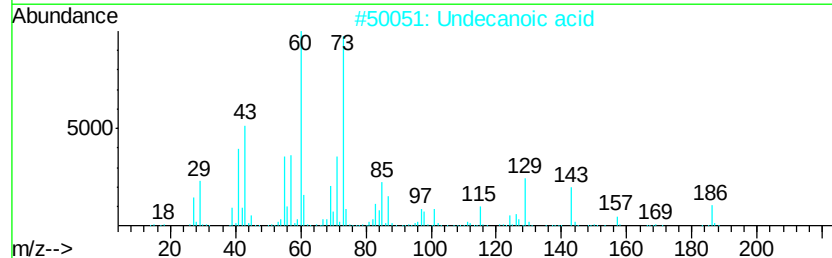
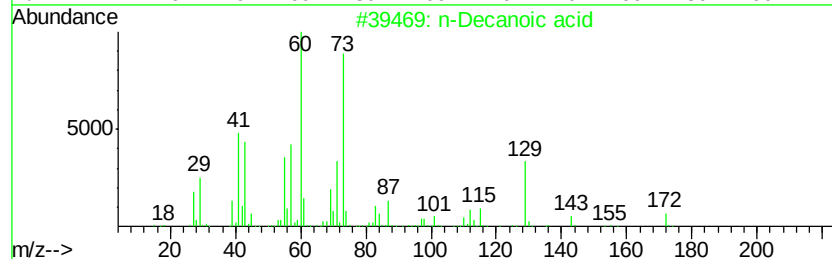
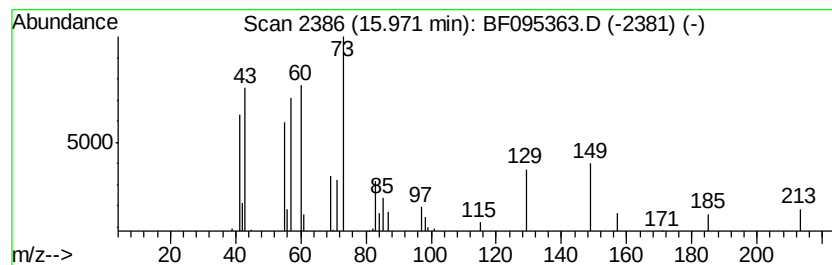
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Peak Number 5 unknown15.97 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.97	2.68 ng	91832	Phenanthrene-d10	15.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	47
2		Undecanoic acid	186	C11H22O2	000112-37-8	35
3		Nonanoic acid	158	C9H18O2	000112-05-0	27
4		.alpha.-D-Glucopyranoside, O-.al...	504	C18H32O16	000597-12-6	22
5		Glucose	180	C6H12O6	000050-99-7	22



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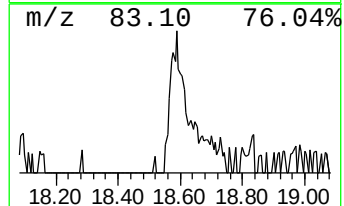
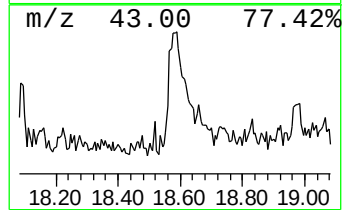
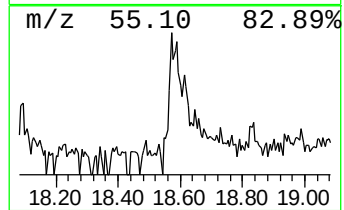
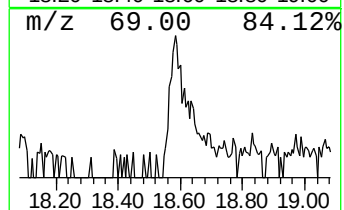
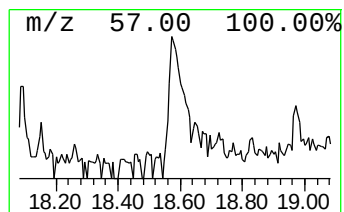
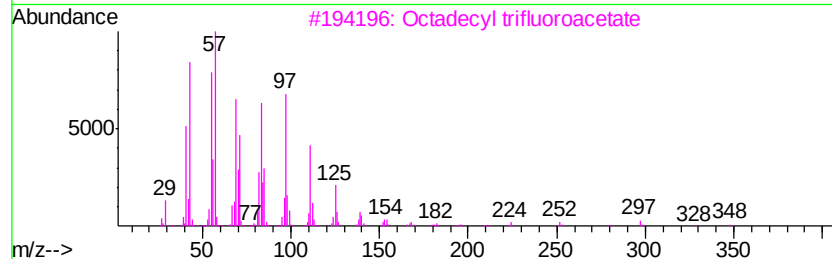
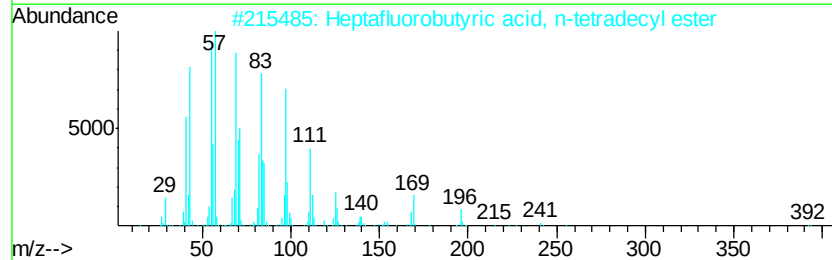
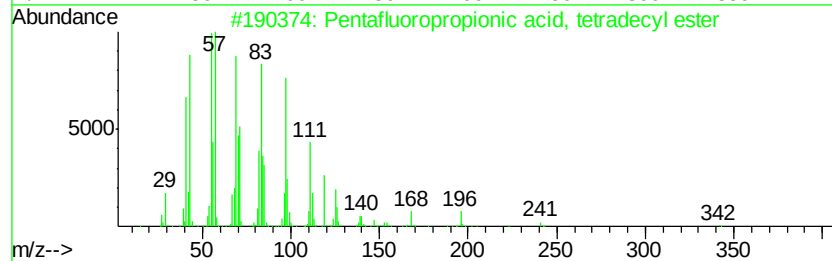
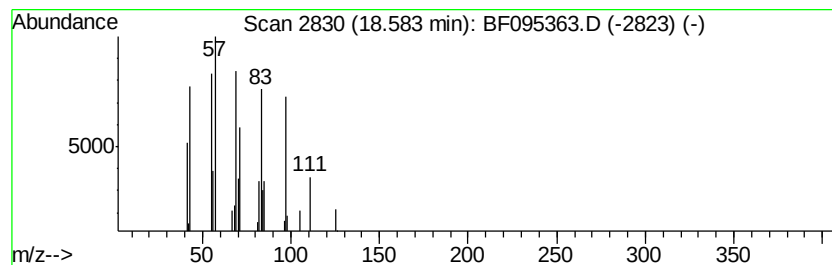
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.58	4.73 ng	96948	Chrysene-d12	18.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90
2		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	90
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	87
4		17-Pentatriacontene	491	C35H70	006971-40-0	80
5		n-Pentadecanol	228	C15H32O	000629-76-5	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.13	8.4	ng	242504	1	7.75	574813	20.0
unknown7.42	7.42	109.3	ng	3140140	1	7.75	574813	20.0
2-Ethylhexyl merc...	12.06	3.1	ng	127205	3	12.61	832156	20.0
unknown15.97	15.97	2.7	ng	91832	4	15.01	685485	20.0
Pentafluoropropio...	18.58	4.7	ng	96948	5	18.69	409505	20.0