

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090116\
 Data File : BF089968.D
 Acq On : 1 Sep 2016 13:35
 Operator : UM/SJ
 Sample : H4617-06
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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:\HPCHEM1\BNA_F\METHODS\8270-BF083116.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	1.632	3	4	13	rVV	299307	624317	9.63%	1.351%
2	1.747	13	14	52	rVB	1963065	5620396	86.70%	12.166%
3	4.764	276	278	283	rBV	336201	450607	6.95%	0.975%
4	5.210	314	317	320	rBV	2583816	2546764	39.29%	5.513%
5	6.273	407	410	412	rBV	2093931	1838192	28.36%	3.979%
6	6.399	419	421	424	rVB	4043653	4233359	65.30%	9.163%
7	6.639	439	442	444	rBV	1108857	1141964	17.62%	2.472%
8	6.799	453	456	458	rBV	3388772	4450865	68.66%	9.634%
9	7.210	488	492	494	rBV	2613647	3832769	59.12%	8.296%
10	7.324	498	502	505	rBV	33268	65683	1.01%	0.142%
11	7.667	528	532	535	rBV	50381	69884	1.08%	0.151%
12	7.839	545	547	552	rBV	83278	79657	1.23%	0.172%
13	7.919	552	554	557	rBV	1691720	1443819	22.27%	3.125%
14	8.879	636	638	646	rVB	260626	261782	4.04%	0.567%
15	9.005	646	649	651	rBV	5596780	6482623	100.00%	14.032%
16	9.393	681	683	685	rBV	168710	142127	2.19%	0.308%
17	9.668	704	707	709	rBV	1540632	1547374	23.87%	3.349%
18	10.090	742	744	748	rVB	142857	139253	2.15%	0.301%
19	10.445	772	775	778	rBV	2708150	2976488	45.91%	6.443%
20	10.673	793	795	799	rVB	86445	81974	1.26%	0.177%
21	11.131	833	835	838	rVB	1276993	1297810	20.02%	2.809%
22	11.691	882	884	885	rBV	63682	79699	1.23%	0.173%
23	11.713	885	886	889	rVB	155174	129040	1.99%	0.279%
24	12.719	971	974	977	rBV	4165484	4092137	63.12%	8.858%
25	13.634	1051	1054	1059	rBV2	138800	186406	2.88%	0.403%
26	13.748	1062	1064	1067	rBV	1349572	1218335	18.79%	2.637%
27	15.097	1179	1182	1185	rBV	1075721	1165990	17.99%	2.524%

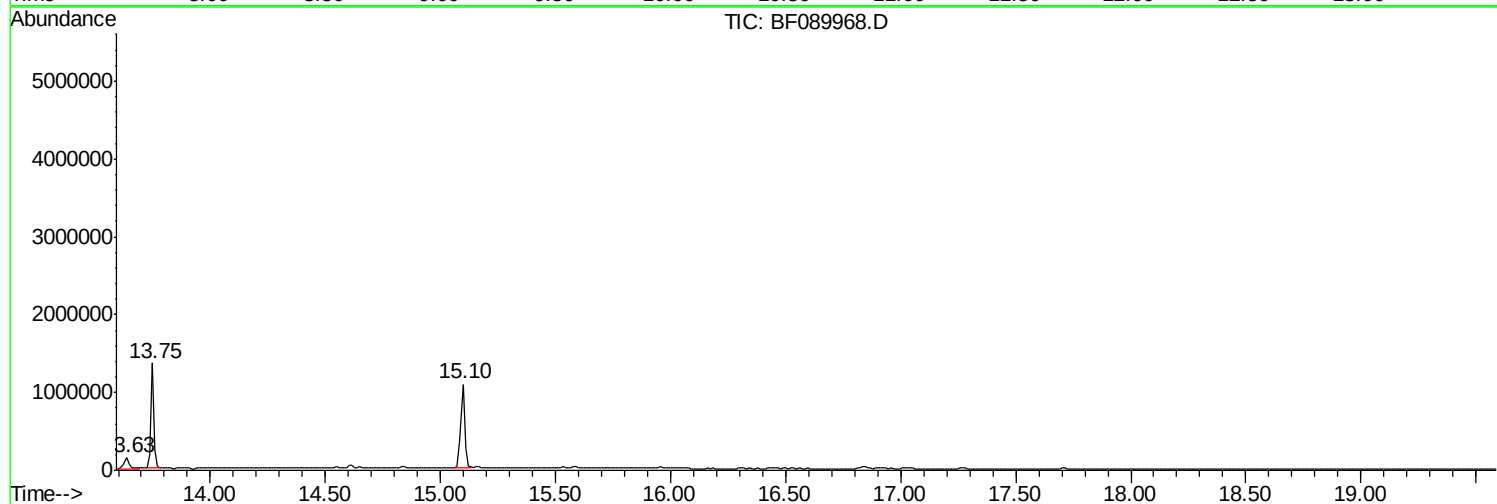
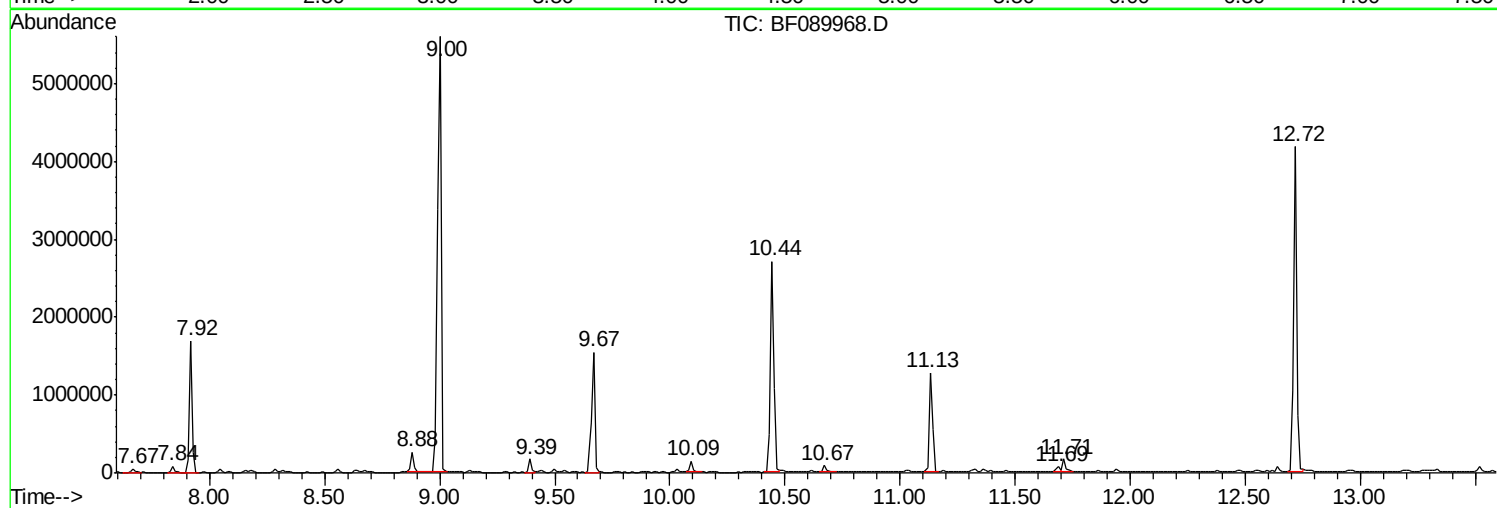
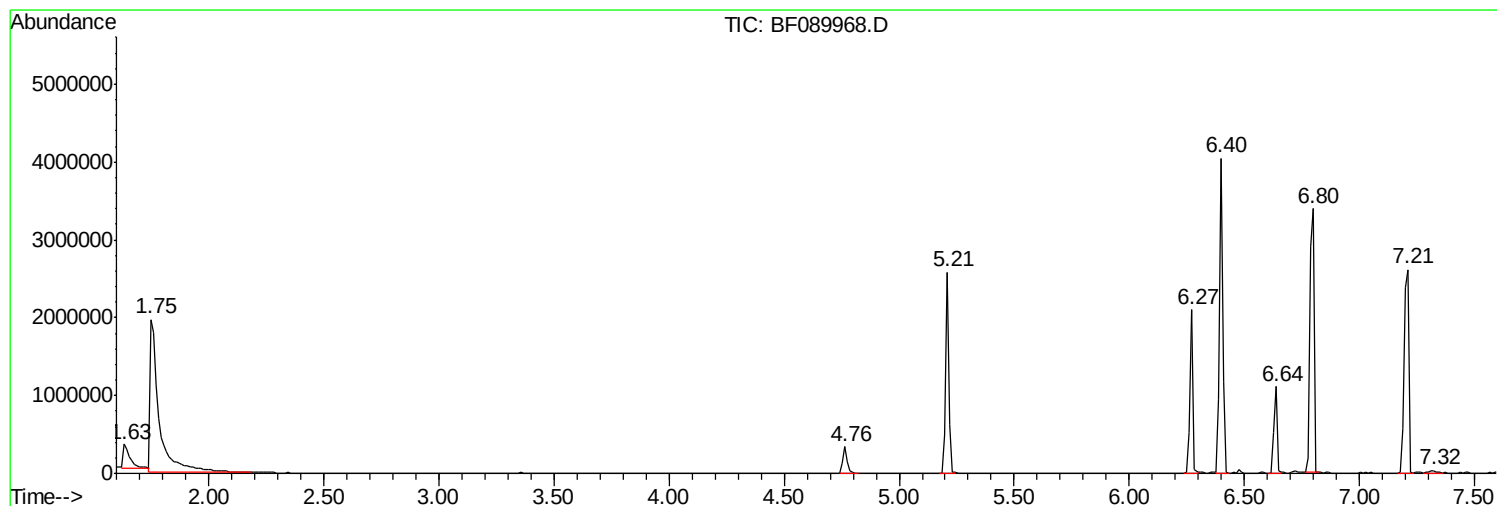
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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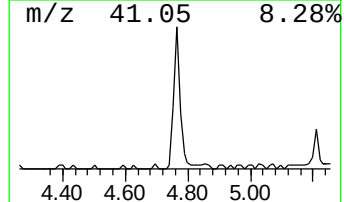
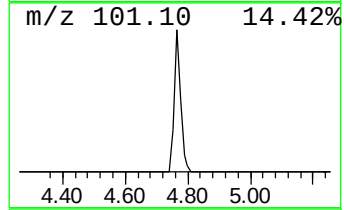
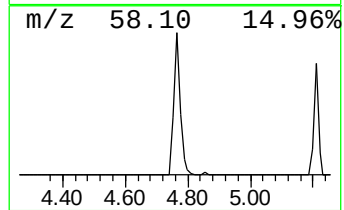
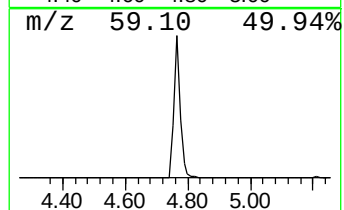
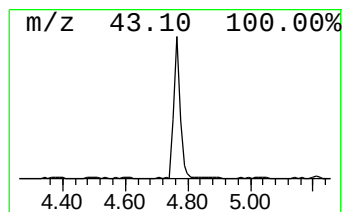
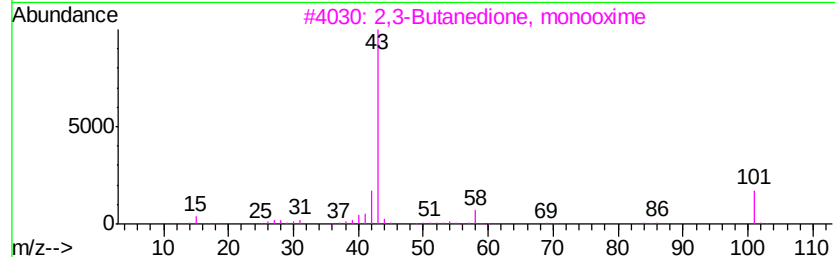
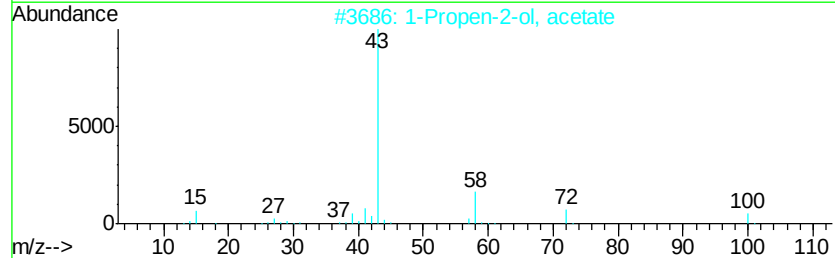
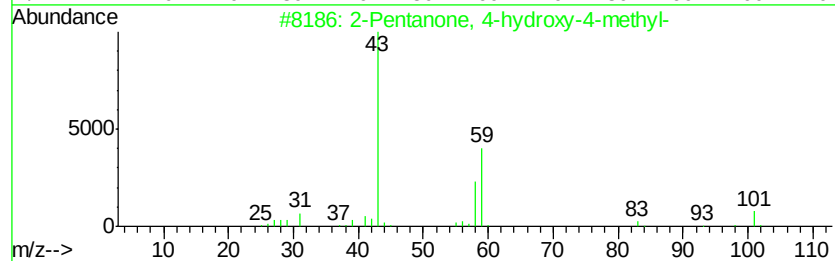
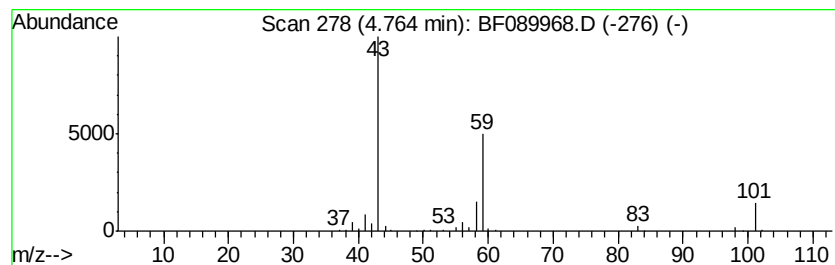
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.76	7.89 ng	450607	1,4-Dichlorobenzene-d4	6.64

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		Butane	58	C4H10	000106-97-8	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	7



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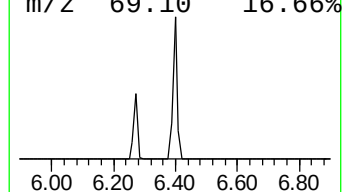
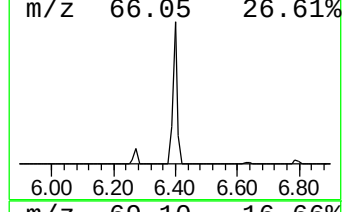
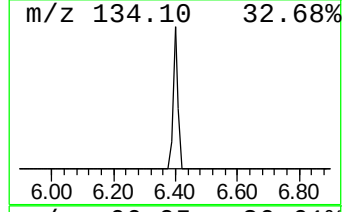
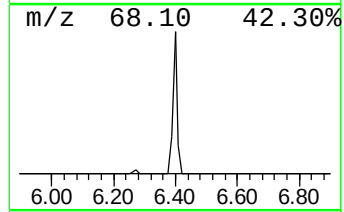
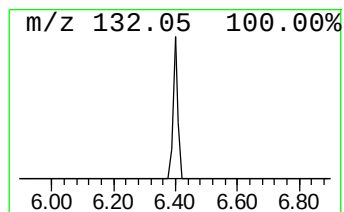
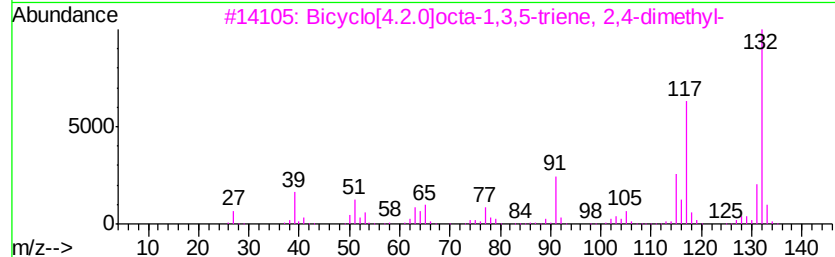
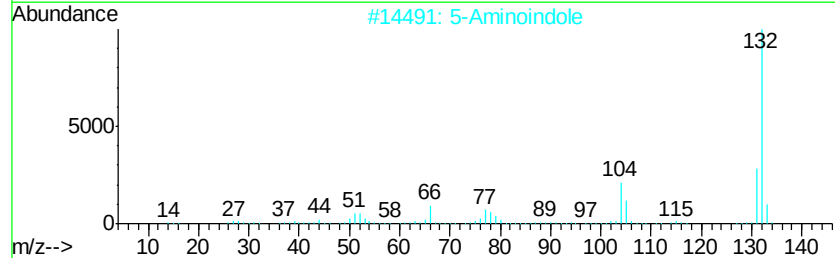
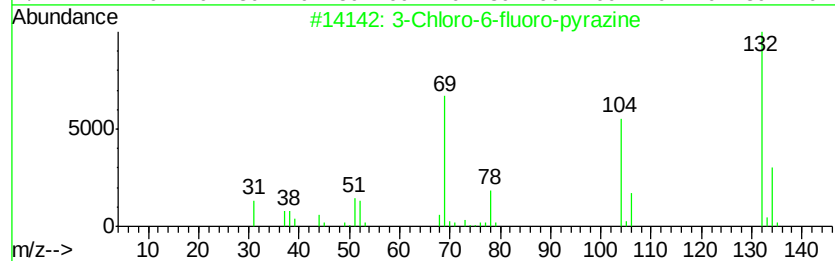
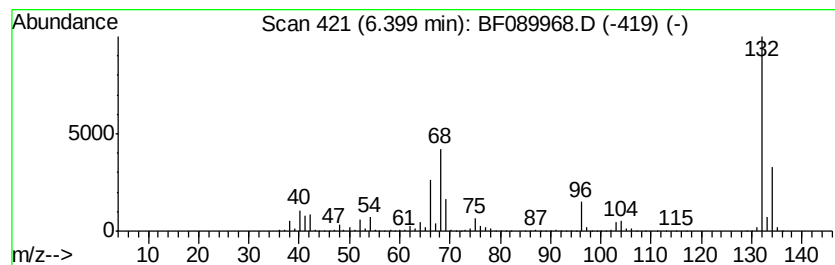
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Peak Number 4 unknown6.40 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	74.14 ng	4233360	1,4-Dichlorobenzene-d4	6.64

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Aminoindole	132	C8H8N2	005192-03-0	12
3			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5			2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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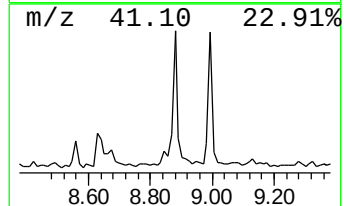
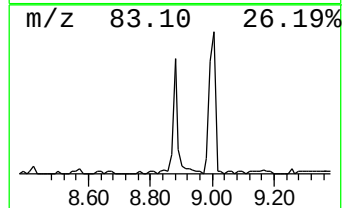
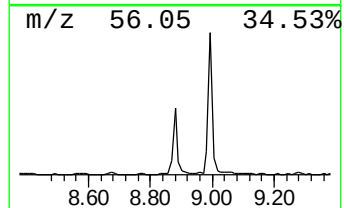
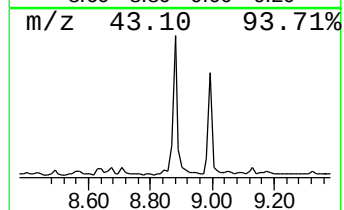
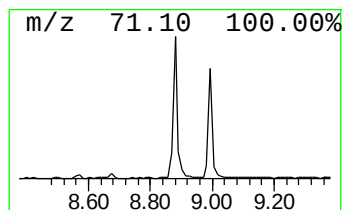
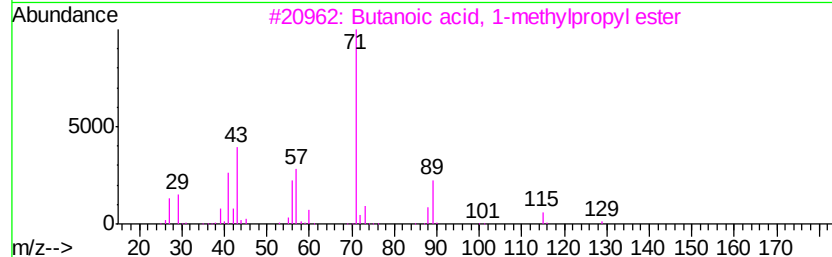
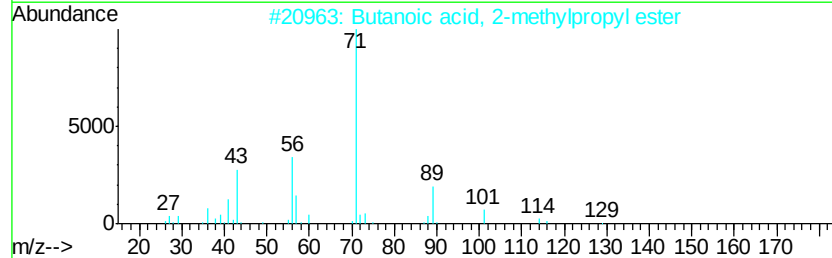
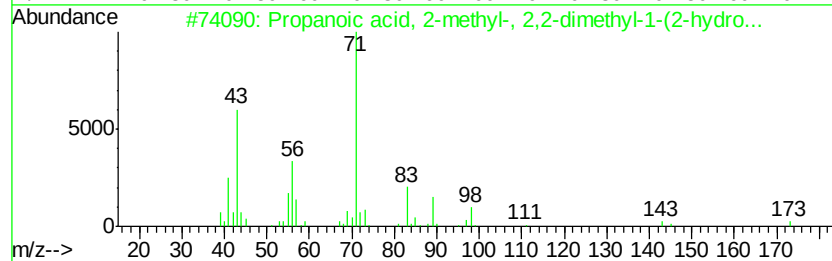
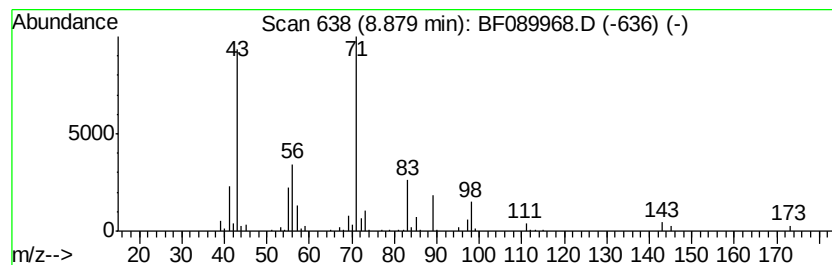
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Peak Number 6 Propanoic acid, 2-methyl-, ... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.88	3.38 ng	261782	Acenaphthene-d10	9.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	90
2		Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	42
3		Butanoic acid, 1-methylpropyl ester	144	C8H16O2	000819-97-6	42
4		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	42
5		Butanoic acid, 1-methyloctyl ester	214	C13H26O2	069727-42-0	40



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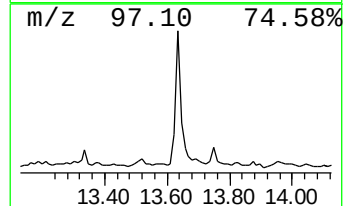
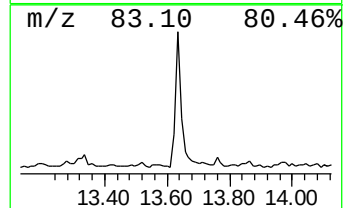
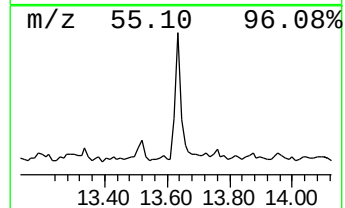
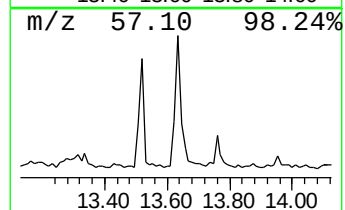
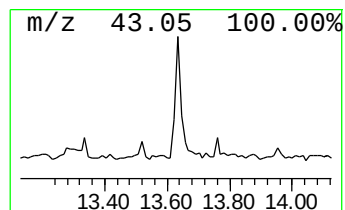
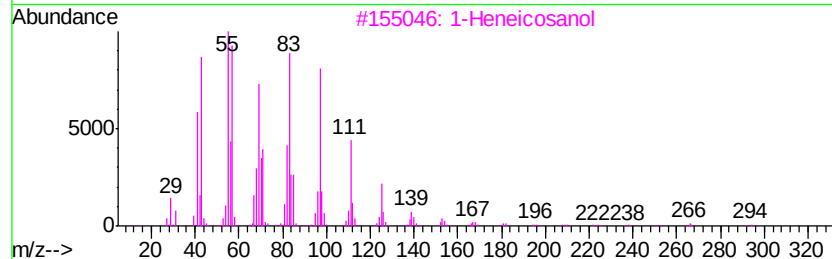
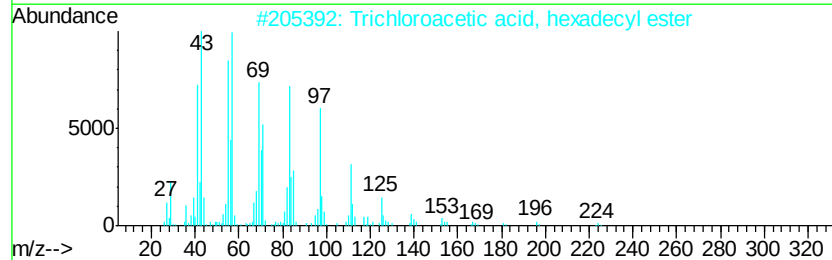
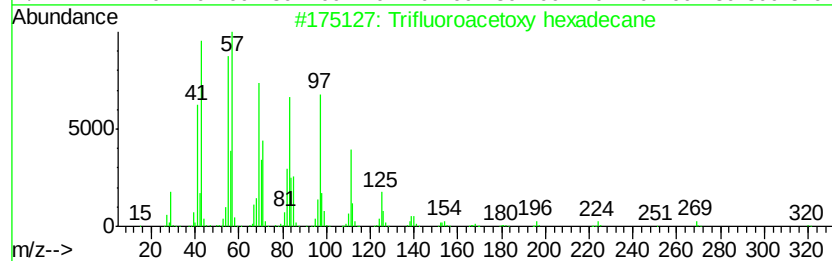
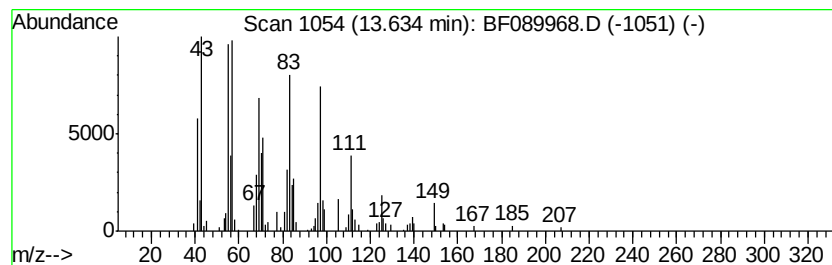
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Peak Number 7 Trifluoroacetoxy hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	3.06 ng	186406	Chrysene-d12	13.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	93
5		Behenic alcohol	326	C22H46O	000661-19-8	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.76	7.9	ng	450607	1	6.64	1141960	20.0
unknown6.40	6.40	74.1	ng	4233360	1	6.64	1141960	20.0
Propanoic acid, 2...	8.88	3.4	ng	261782	3	9.67	1547370	20.0
Trifluoroacetoxy ...	13.63	3.1	ng	186406	5	13.75	1218340	20.0