

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090816\
 Data File : BF090033.D
 Acq On : 8 Sep 2016 19:20
 Operator : UM/SJ
 Sample : H4704-04
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-4-6.5-7.5

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	1.724	10	12	62	rVB	4519002	11890211	100.00%	22.837%
2	4.730	272	275	285	rBV	543953	1017950	8.56%	1.955%
3	5.176	311	314	327	rBV	3376505	3945177	33.18%	7.577%
4	6.250	404	408	410	rBV	3366461	4320888	36.34%	8.299%
5	6.365	415	418	420	rBV	4018527	4008194	33.71%	7.698%
6	6.593	436	438	449	rVB	797159	1080774	9.09%	2.076%
7	6.753	449	452	455	rBV	3295817	3109108	26.15%	5.971%
8	7.165	485	488	496	rBV	2152191	2508318	21.10%	4.818%
9	7.290	496	499	508	rVB	94300	188533	1.59%	0.362%
10	7.885	548	551	553	rBV	1516587	1377913	11.59%	2.646%
11	8.971	643	646	648	rBV	3510836	4761400	40.04%	9.145%
12	9.359	678	680	683	rBV	1232155	1314411	11.05%	2.525%
13	9.633	701	704	706	rBV	1429222	1622926	13.65%	3.117%
14	10.411	769	772	775	rBV	2364181	2591502	21.80%	4.977%
15	10.548	783	784	789	rVB	84316	147745	1.24%	0.284%
16	11.096	830	832	843	rVB	1343840	1594736	13.41%	3.063%
17	12.685	968	971	973	rBV	3827566	3933948	33.09%	7.556%
18	13.588	1048	1050	1059	rBV	143161	210987	1.77%	0.405%
19	13.714	1059	1061	1069	rVV	1206351	1342330	11.29%	2.578%
20	15.051	1175	1178	1182	rBV	908803	1098963	9.24%	2.111%

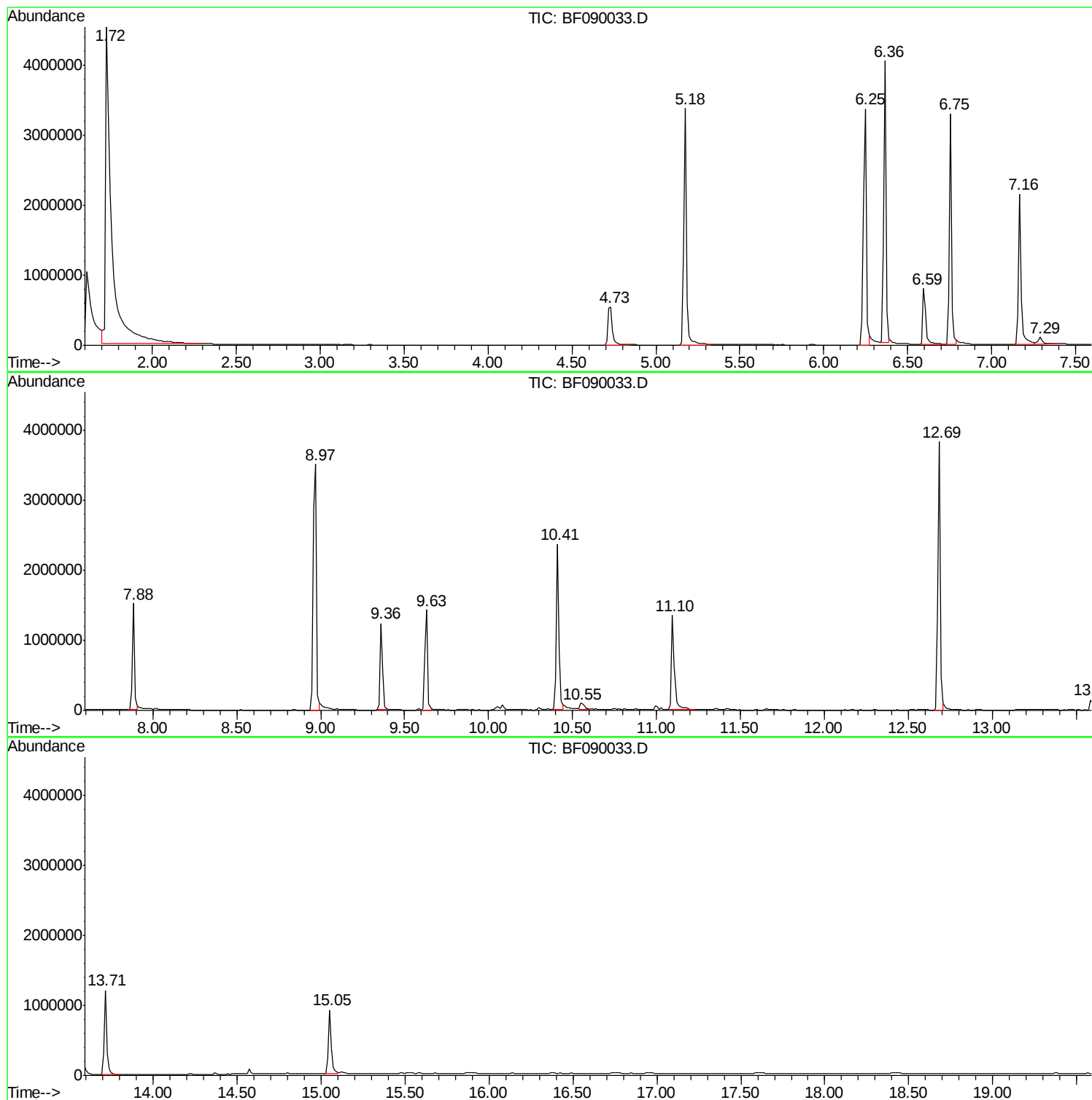
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF083116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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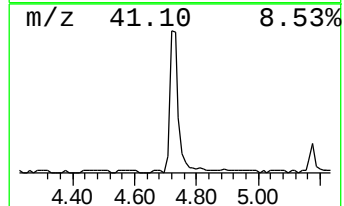
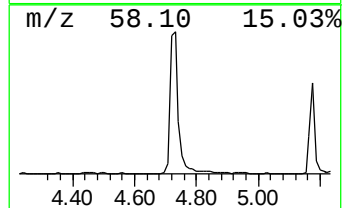
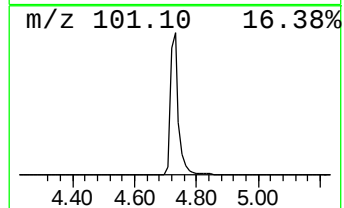
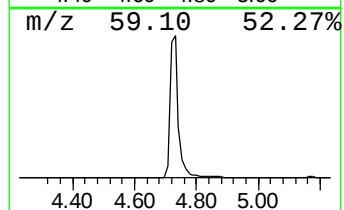
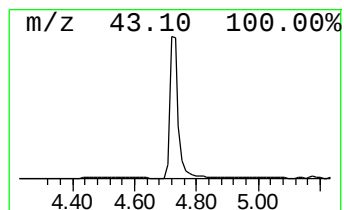
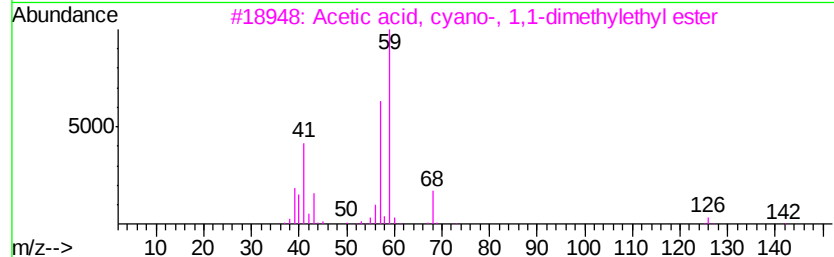
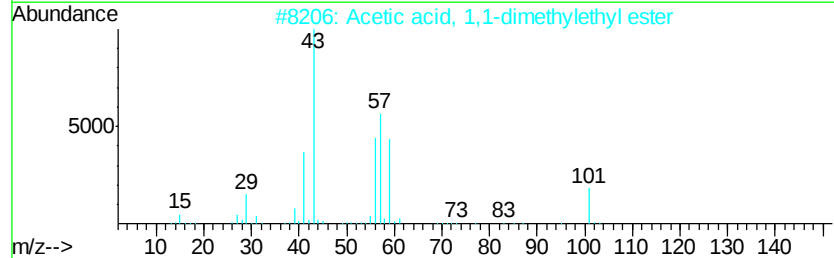
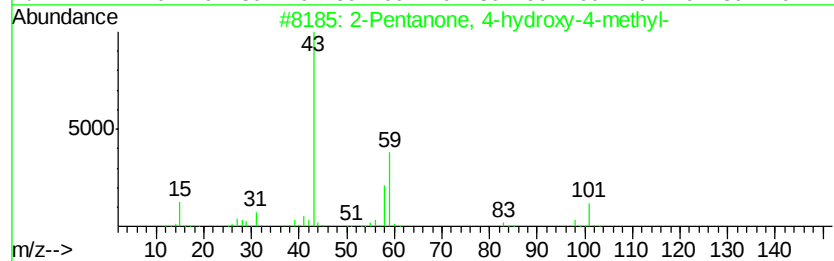
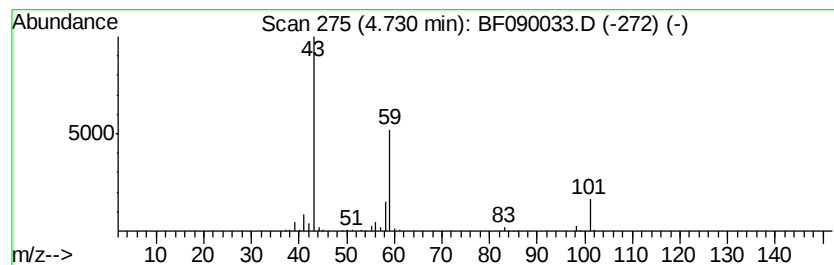
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.73	18.84 ng	1017950	1,4-Dichlorobenzene-d4	6.59

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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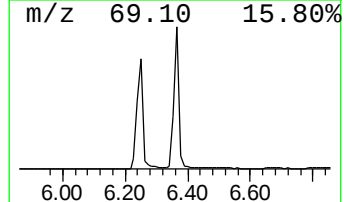
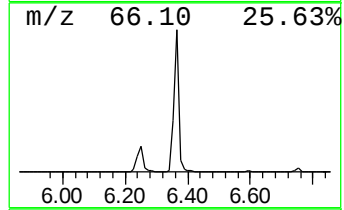
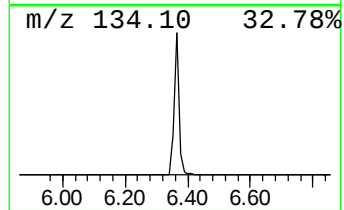
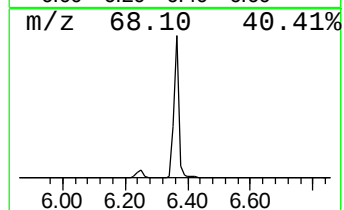
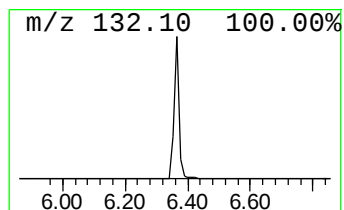
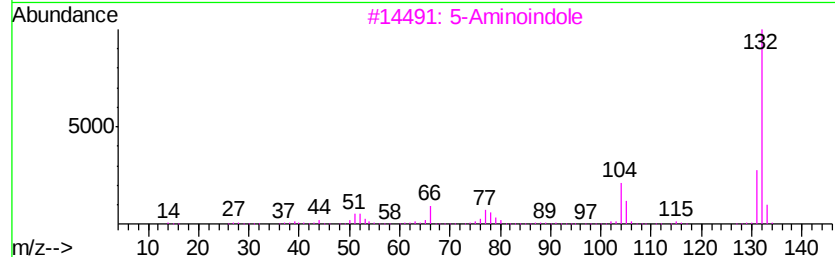
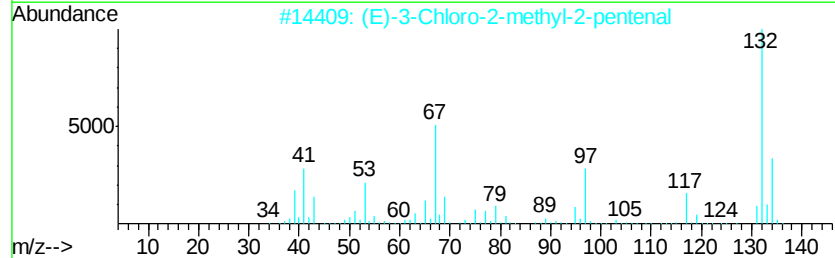
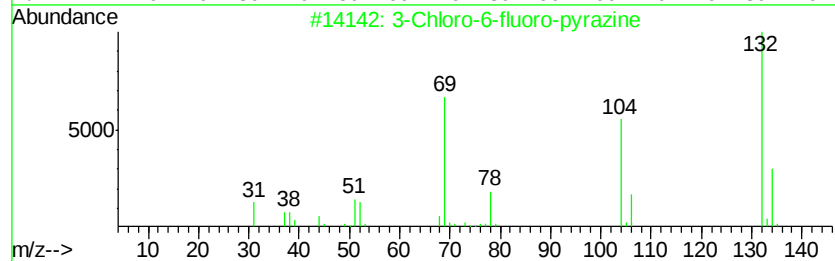
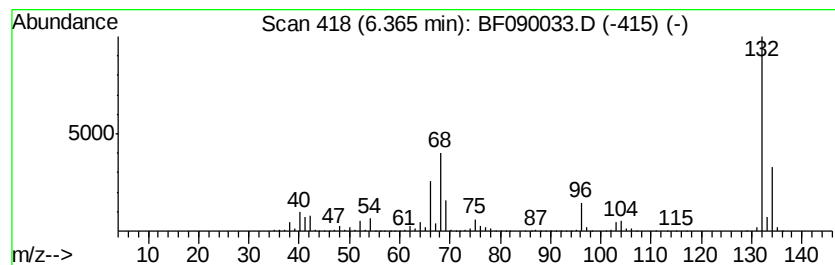
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Peak Number 3 unknown6.36 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.36	74.17 ng	4008190	1,4-Dichlorobenzene-d4	6.59

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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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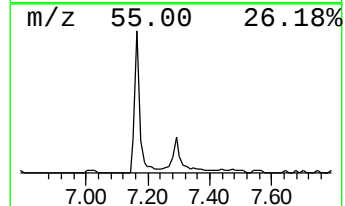
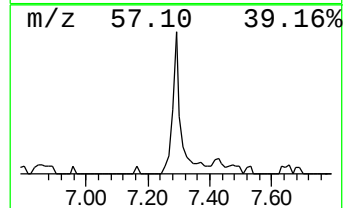
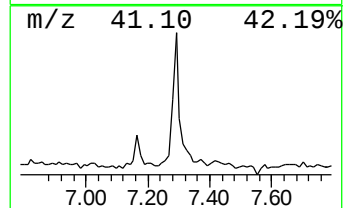
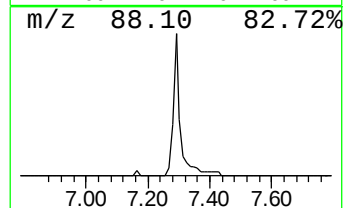
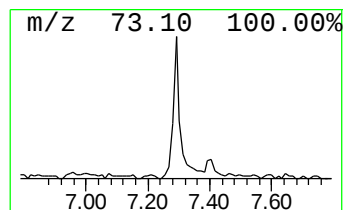
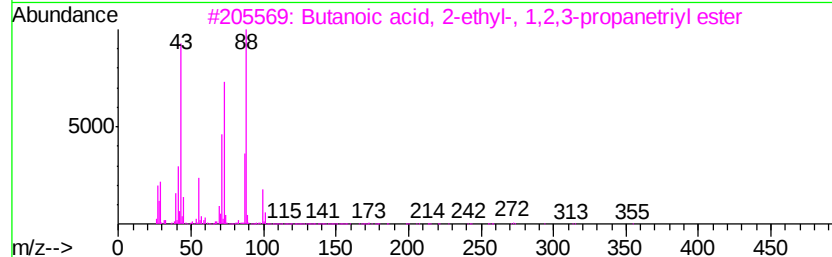
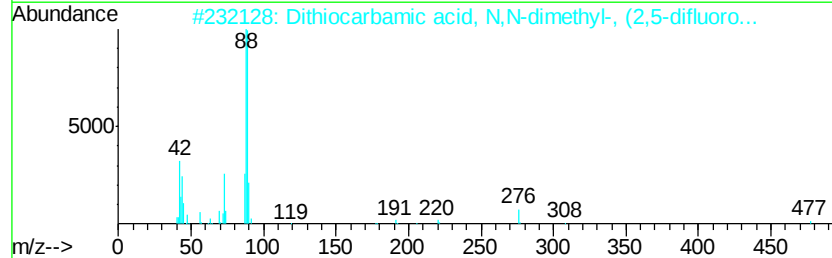
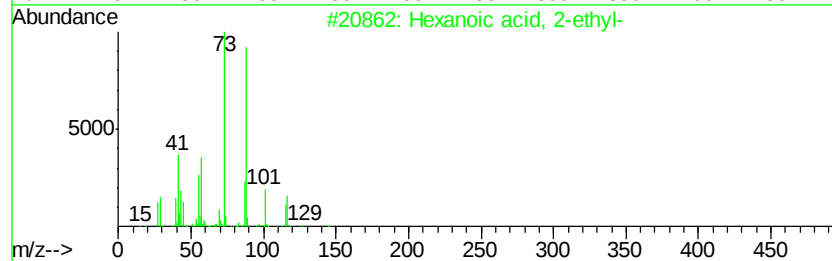
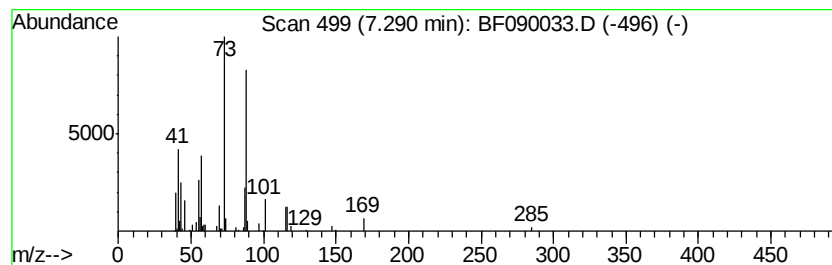
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Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.29	2.74 ng	188533	Naphthalene-d8	7.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	86
2		Dithiocarbamic acid, N,N-dimethyl...	477	C13H12F9N3S3	1000268-72-7	45
3		Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	42
4		3-Aza-2-oxabicyclo[2.2.2]oct-5-e...	267	C10H12F3N04	102698-35-1	40
5		1,4-Dioxane	88	C4H8O2	000123-91-1	38



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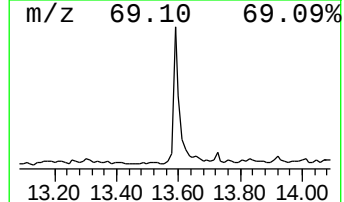
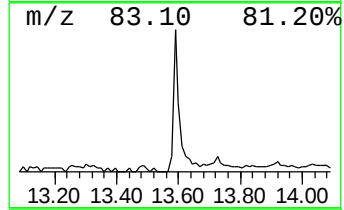
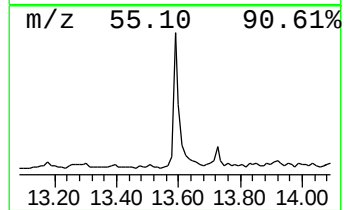
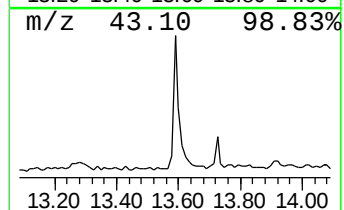
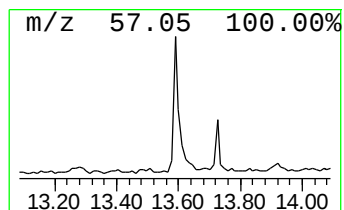
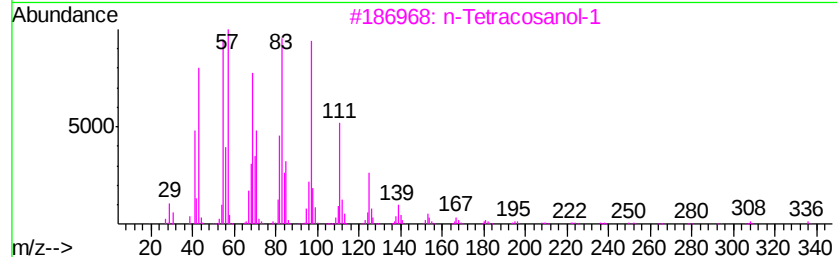
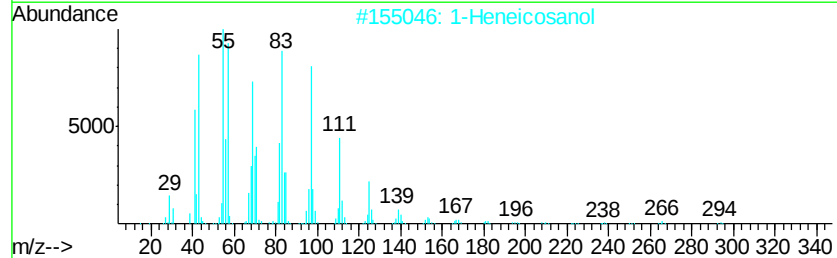
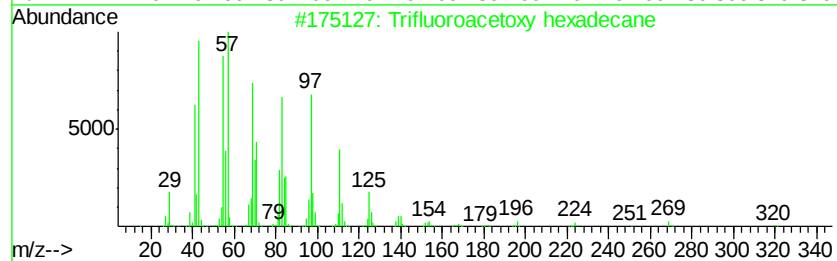
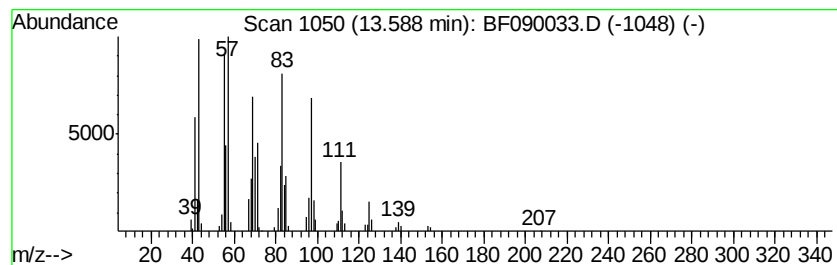
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.59	3.14 ng	210987	Chrysene-d12	13.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		1-Heneicosanol	312	C21H44O	015594-90-8	94
3		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.73	18.8	ng	1017950	1	6.59	1080770	20.0
unknown6.36	6.36	74.2	ng	4008190	1	6.59	1080770	20.0
Hexanoic acid, 2-...	7.29	2.7	ng	188533	2	7.88	1377910	20.0
Trifluoroacetoxy ...	13.59	3.1	ng	210987	5	13.71	1342330	20.0