

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF090115\
 Data File : BF081331.D
 Acq On : 2 Sep 2015 5:22
 Operator : UM/IZ
 Sample : G3480-07
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 COFF-3-14(0-2)

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-BF090115.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	4.456	246	251	262	rVB	661308	1332044	61.21%	7.628%
2	4.936	291	293	296	rBV	1332538	1886994	86.70%	10.806%
3	6.056	388	391	393	rBV	1829576	2176357	100.00%	12.463%
4	6.159	397	400	402	rBV	1440025	1916972	88.08%	10.978%
5	6.387	418	420	422	rBV	454308	379489	17.44%	2.173%
6	6.547	431	434	436	rBV	1014855	1265841	58.16%	7.249%
7	6.959	468	470	473	rBV	861727	1205946	55.41%	6.906%
8	7.679	530	533	535	rBV	471064	480654	22.09%	2.752%
9	8.753	625	627	630	rBV	1242617	1671476	76.80%	9.572%
10	9.165	660	663	665	rVB	352872	343383	15.78%	1.966%
11	9.416	682	685	687	rVB	592167	516438	23.73%	2.957%
12	10.193	751	753	756	rBV2	894565	1001455	46.02%	5.735%
13	10.353	764	767	770	rBV	18931	25599	1.18%	0.147%
14	10.879	811	813	815	rBV	652581	536115	24.63%	3.070%
15	11.222	840	843	845	rVB	16538	21938	1.01%	0.126%
16	11.451	861	863	867	rBV2	63643	74979	3.45%	0.429%
17	12.468	949	952	954	rBV	1604352	1509269	69.35%	8.643%
18	13.382	1030	1032	1039	rBV	145812	280855	12.90%	1.608%
19	13.485	1039	1041	1044	rVV	462975	421376	19.36%	2.413%
20	14.011	1085	1087	1093	rBV3	11355	25849	1.19%	0.148%
21	14.800	1153	1156	1158	rBV	309334	320568	14.73%	1.836%
22	15.245	1193	1195	1209	rVB3	21299	68990	3.17%	0.395%

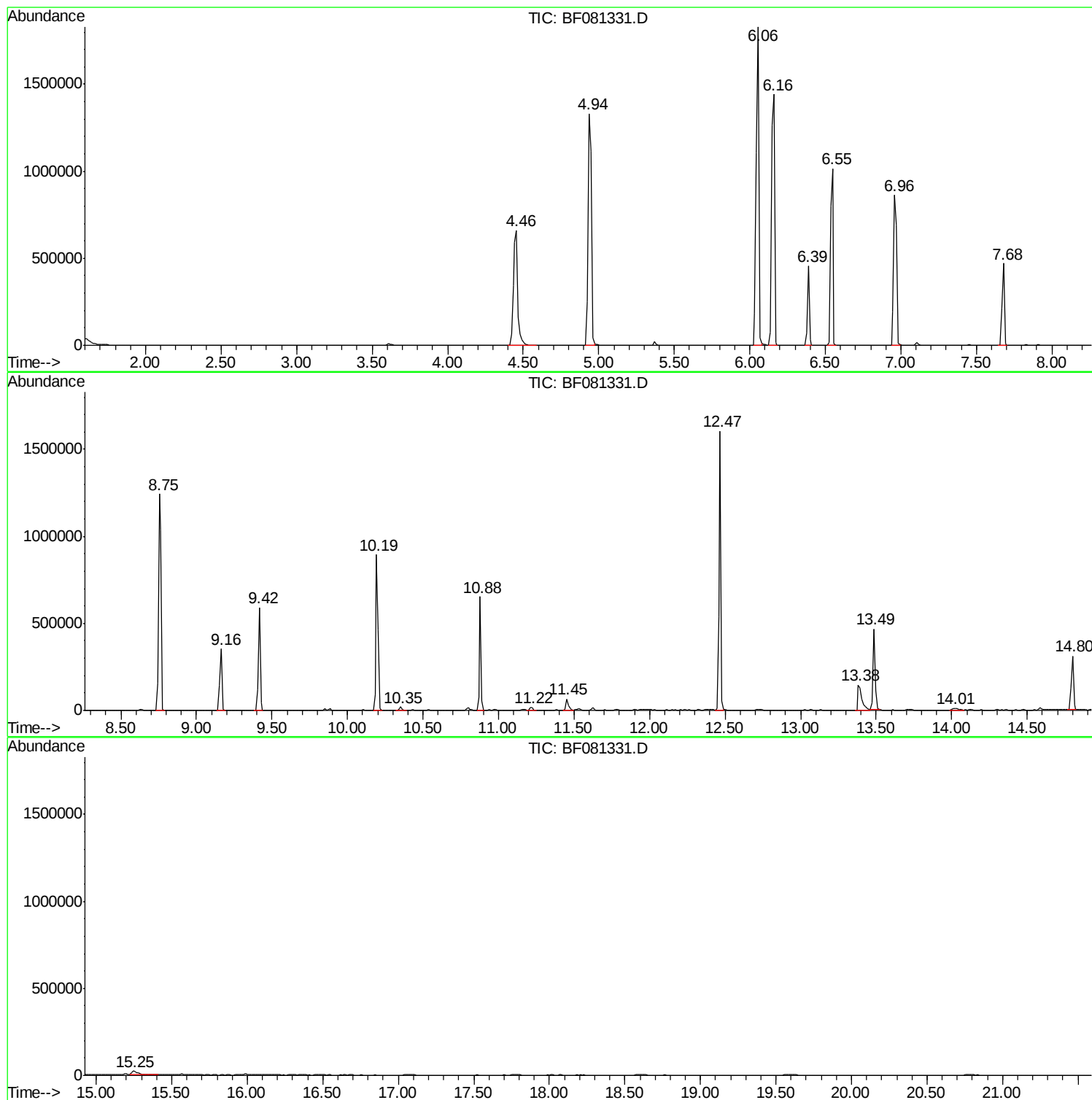
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF090115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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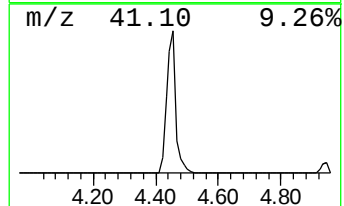
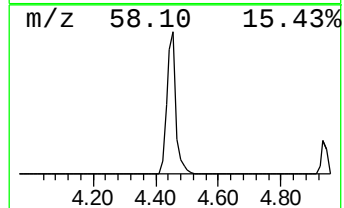
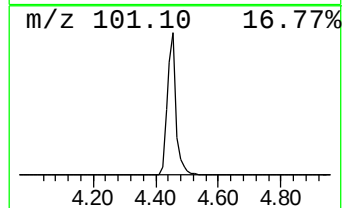
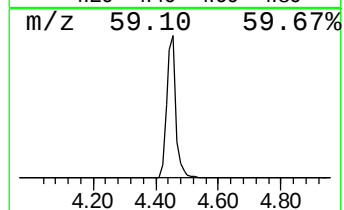
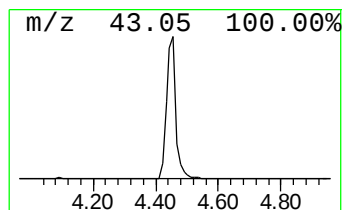
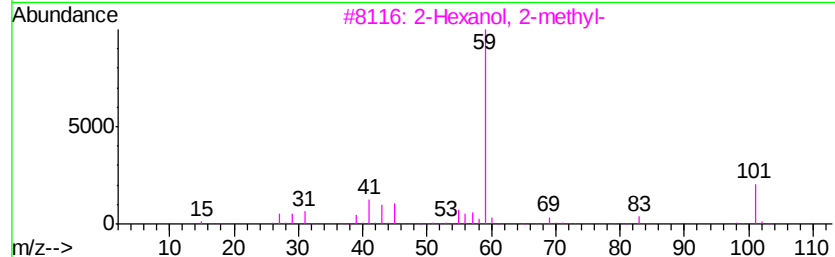
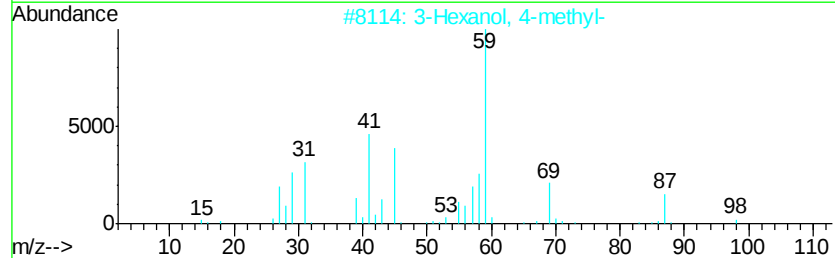
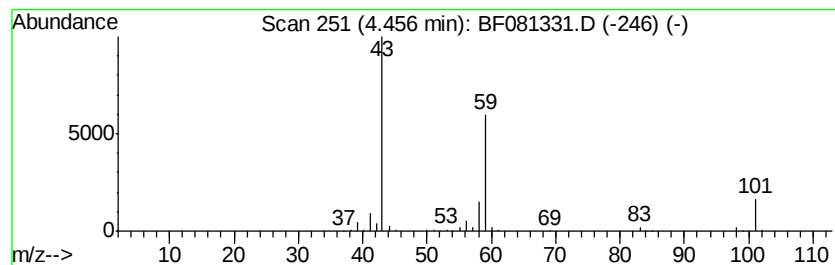
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.46	70.20 ng	1332040	1,4-Dichlorobenzene-d4	6.39

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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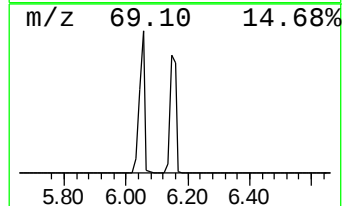
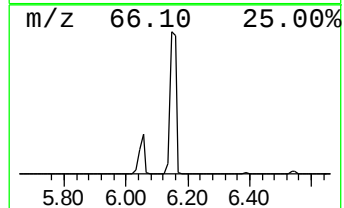
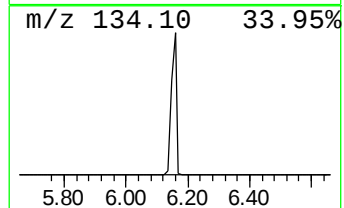
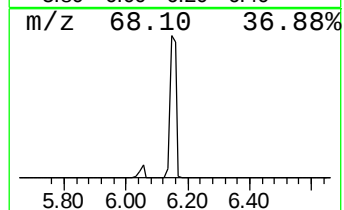
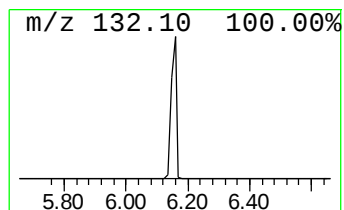
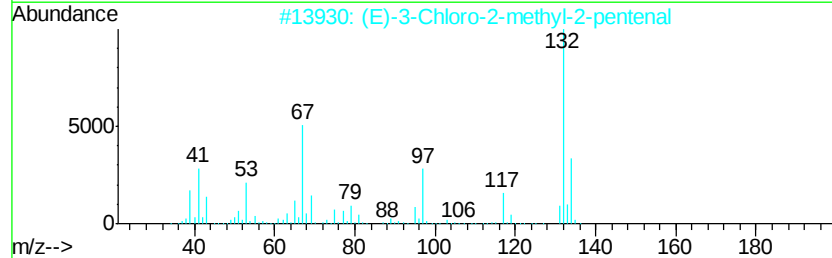
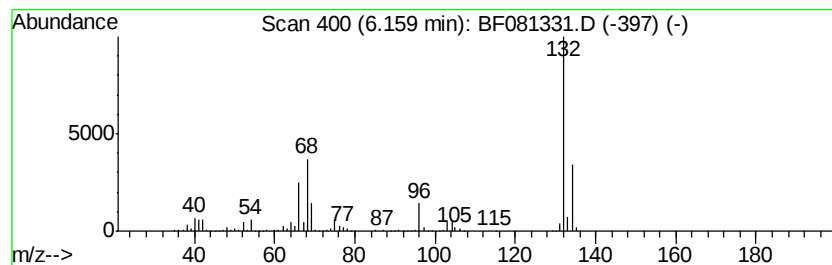
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.16 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.16	101.03 ng	1916970	1,4-Dichlorobenzene-d4	6.39

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
4		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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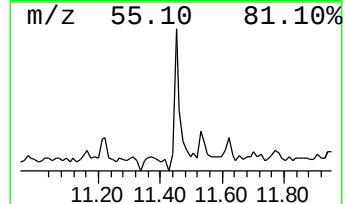
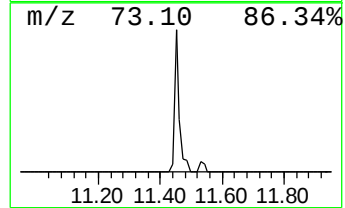
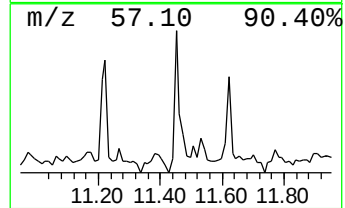
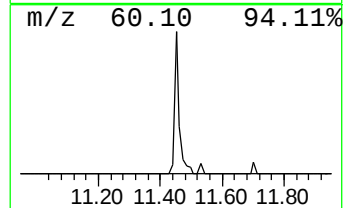
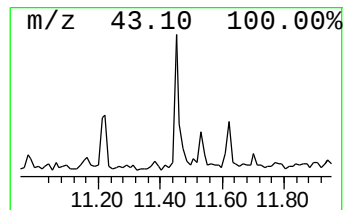
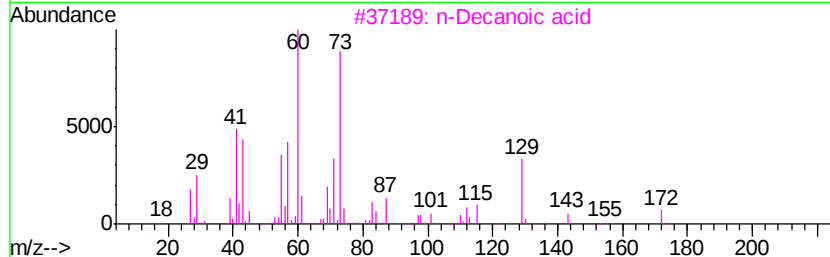
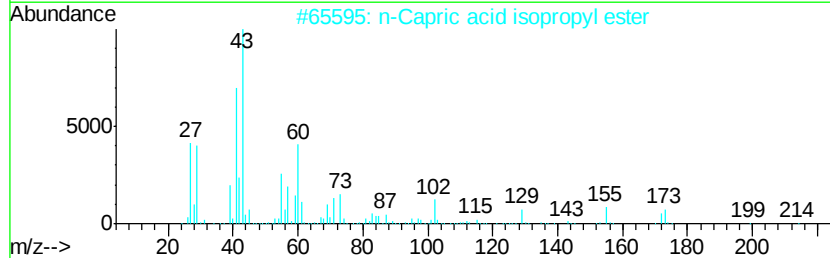
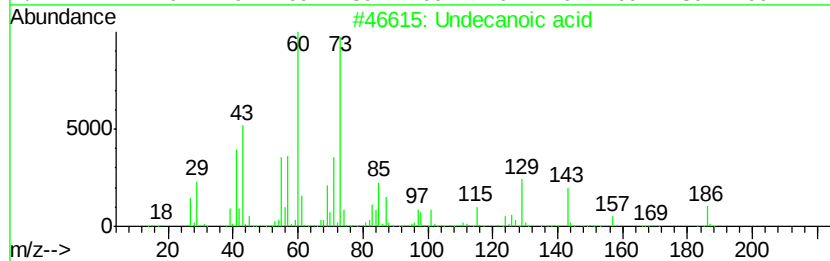
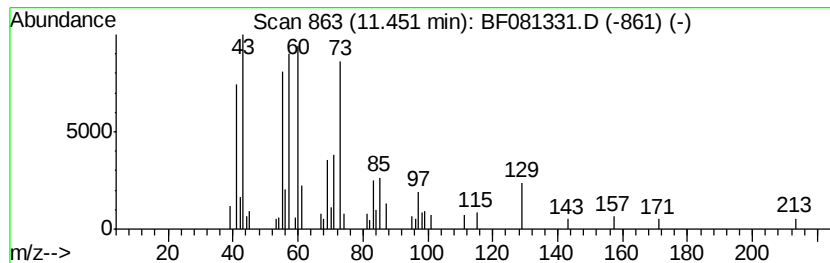
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Peak Number 4 Undecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.45	2.80 ng	74979	Phenanthrene-d10	10.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecanoic acid	186	C11H22O2	000112-37-8	64
2			n-Capric acid isopropyl ester	214	C13H26O2	002311-59-3	53
3			n-Decanoic acid	172	C10H20O2	000334-48-5	50
4			Dodecanoic acid	200	C12H24O2	000143-07-7	50
5			.beta.-D-Ribopyranoside, methyl	164	C6H12O5	017289-61-1	38



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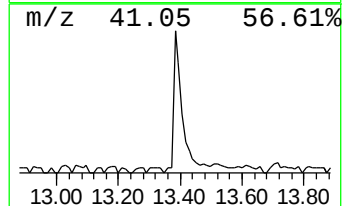
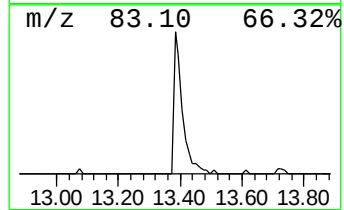
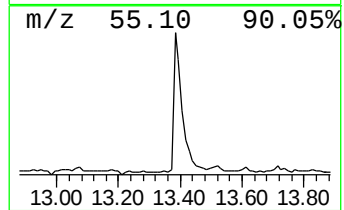
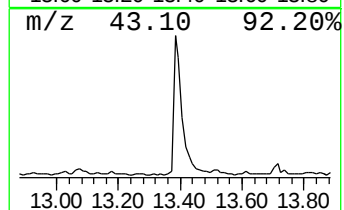
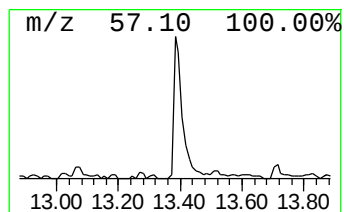
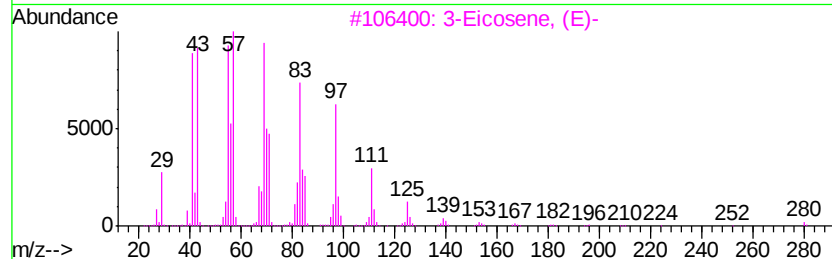
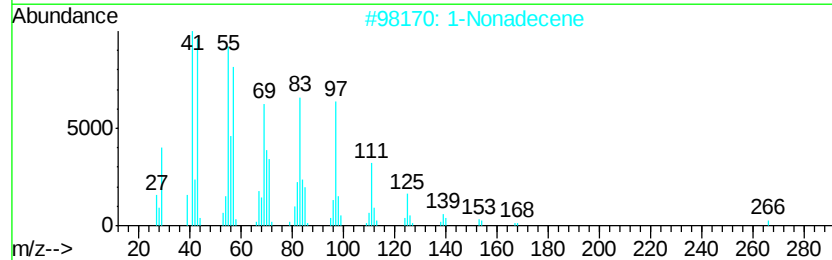
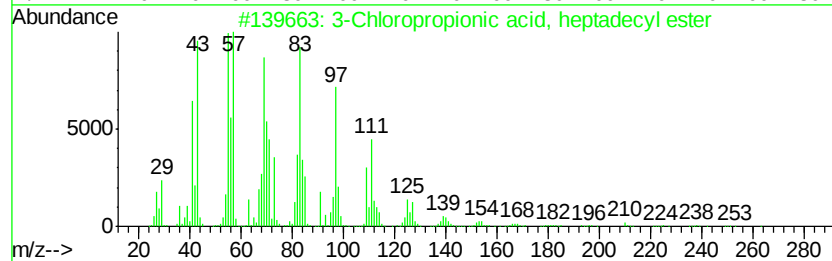
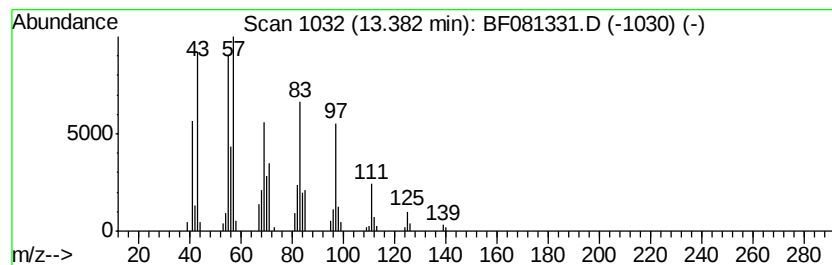
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Peak Number 5 3-Chloropropionic acid, hep... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.38	13.33 ng	280855	Chrysene-d12	13.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
2		1-Nonadecene	266	C19H38	018435-45-5	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	87
4		9-Eicosene, (E)-	280	C20H40	074685-29-3	87
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	81



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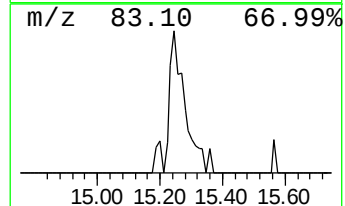
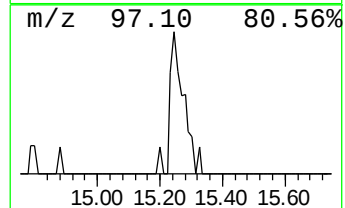
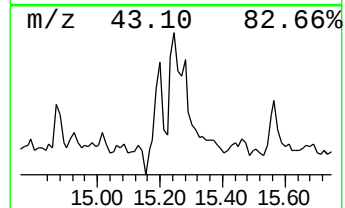
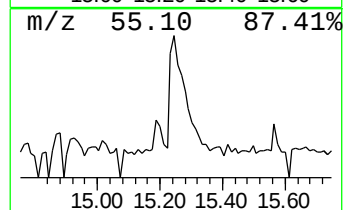
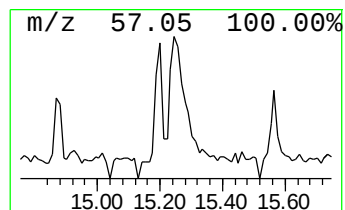
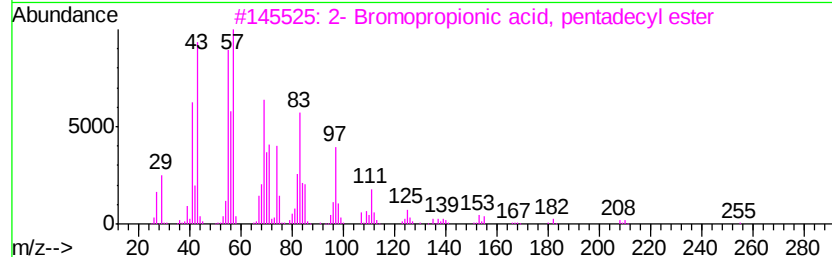
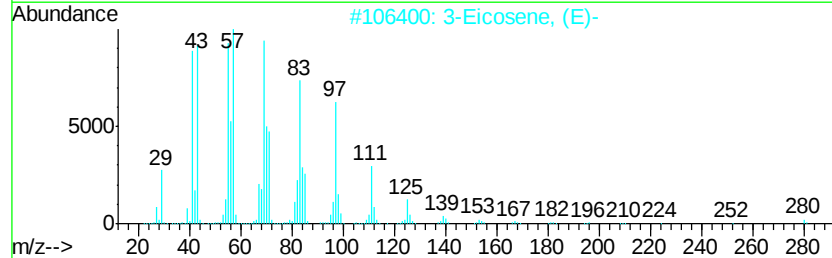
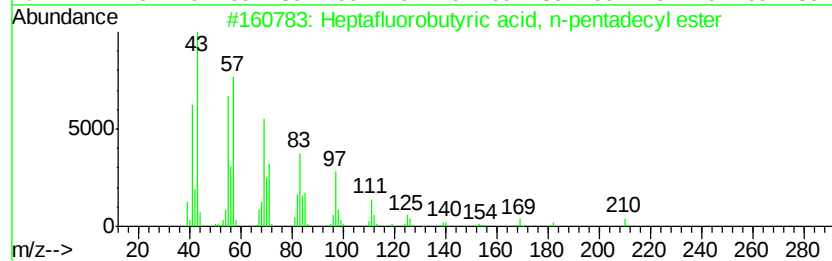
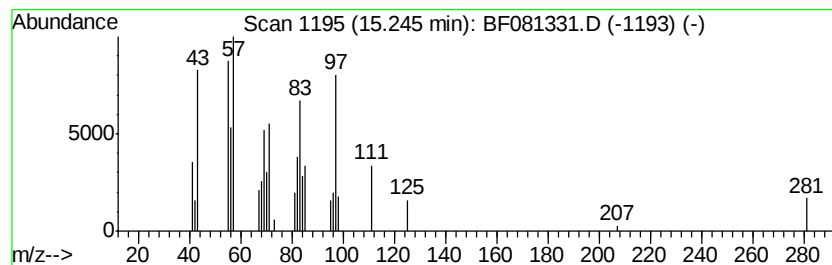
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Peak Number 6 Heptafluorobutyric acid, n-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.25	4.30 ng	68990	Perylene-d12	14.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	86
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	80
3		2- Bromopropionic acid, pentadec...	362	C18H35BrO2	1000292-44-2	80
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	80
5		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.46	70.2	ng	1332040	1	6.39	379489	20.0
unknown6.16	6.16	101.0	ng	1916970	1	6.39	379489	20.0
Undecanoic acid	11.45	2.8	ng	74979	4	10.88	536115	20.0
3-Chloropropionic...	13.38	13.3	ng	280855	5	13.49	421376	20.0
Heptafluorobutyri...	15.25	4.3	ng	68990	6	14.80	320568	20.0