

Data Path : Z:\HPCHEM1\BNA F\DATA\BF122916\
 Data File : BF092035.D
 Acq On : 29 Dec 2016 20:25
 Operator : UM/SJ
 Sample : H6301-06
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-14

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-BF122116.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	4.830	238	240	248	rBV	635253	743825	13.92%	1.994%
2	5.299	278	281	283	rBV	2209176	2428390	45.45%	6.510%
3	6.350	370	373	375	rBV	1665120	1476662	27.64%	3.958%
4	6.464	380	383	385	rBV	4326851	3864294	72.32%	10.359%
5	6.693	401	403	405	rBV	849324	916888	17.16%	2.458%
6	6.842	414	416	419	rBV	2715780	3298981	61.74%	8.843%
7	7.265	450	453	455	rBV	2554348	3154559	59.04%	8.456%
8	7.973	513	515	518	rBV	1351848	1234365	23.10%	3.309%
9	9.059	607	610	612	rBV	5559141	5343167	100.00%	14.323%
10	9.459	642	645	646	rBV	57821	65229	1.22%	0.175%
11	9.722	666	668	671	rBV	1161105	1380552	25.84%	3.701%
12	10.168	703	707	710	rBV3	39934	60139	1.13%	0.161%
13	10.225	710	712	717	rVB2	92132	108067	2.02%	0.290%
14	10.522	735	738	740	rBV	2864366	3430896	64.21%	9.197%
15	10.648	746	749	752	rVB	43888	73918	1.38%	0.198%
16	11.208	796	798	800	rBV	1750147	1509081	28.24%	4.045%
17	11.756	844	846	848	rBV	194727	218305	4.09%	0.585%
18	12.534	913	914	917	rBV2	135443	177556	3.32%	0.476%
19	12.797	934	937	940	rBV	4700534	5142013	96.24%	13.784%
20	13.699	1013	1016	1021	rBV3	85573	149211	2.79%	0.400%
21	13.837	1026	1028	1031	rBV	1521639	1426878	26.70%	3.825%
22	15.220	1146	1149	1152	rBV	913549	1101515	20.62%	2.953%

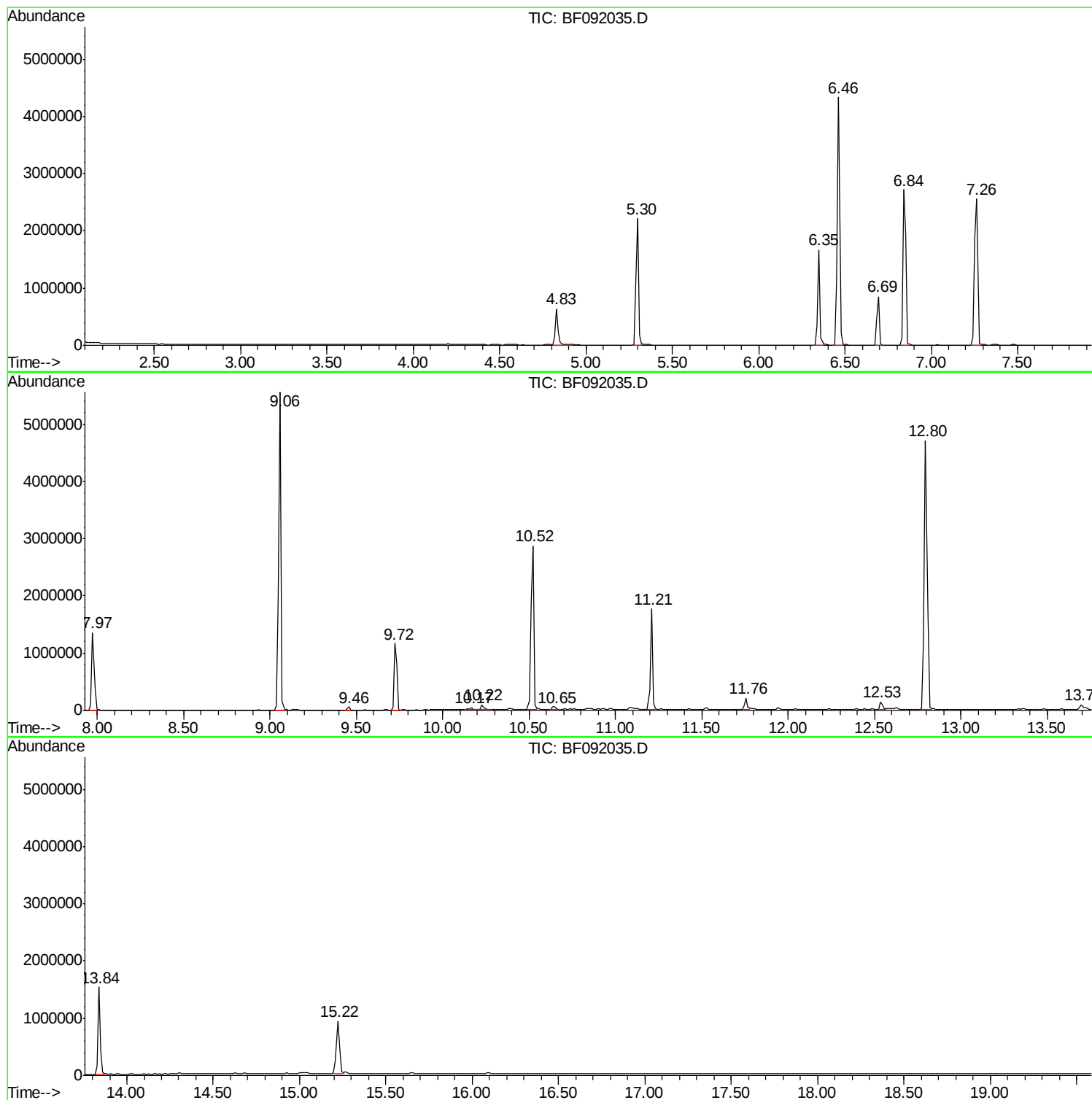
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF122116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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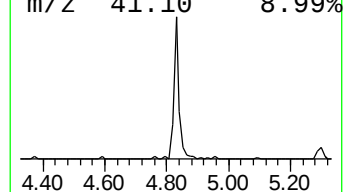
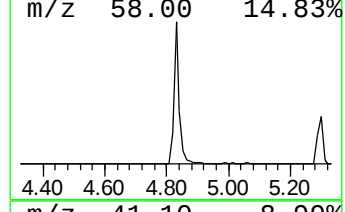
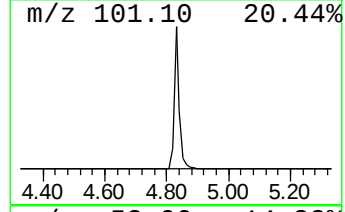
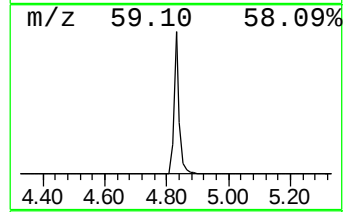
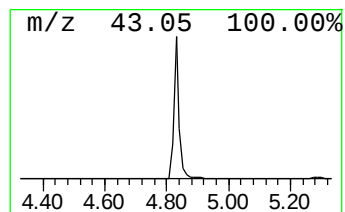
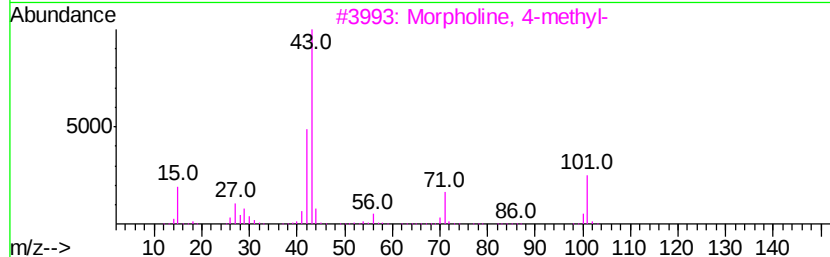
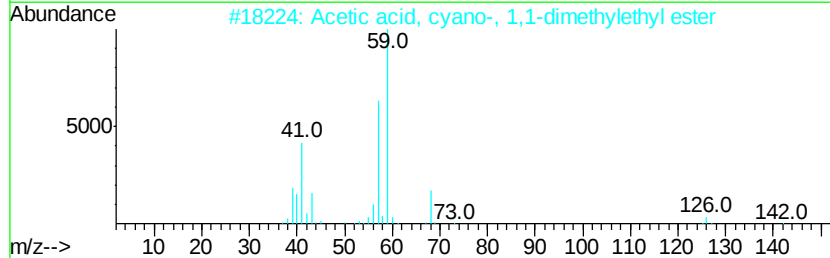
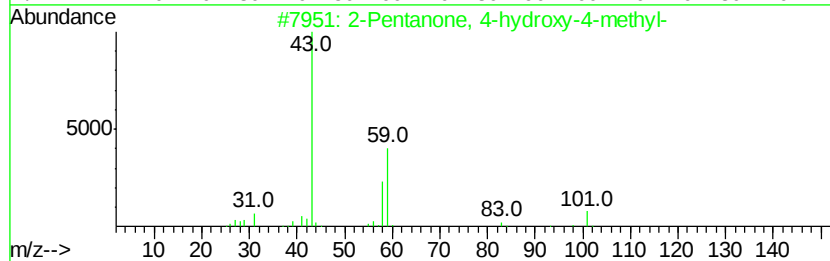
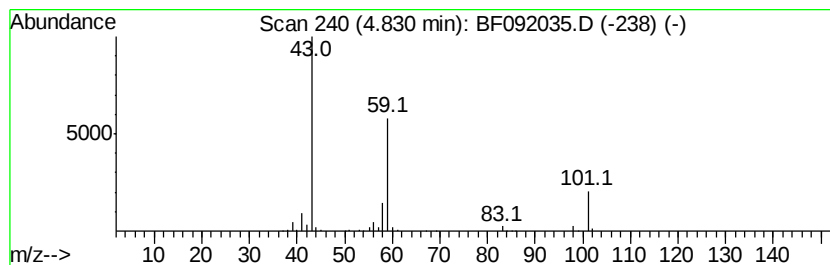
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	16.23 ng	743825	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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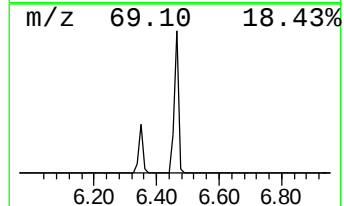
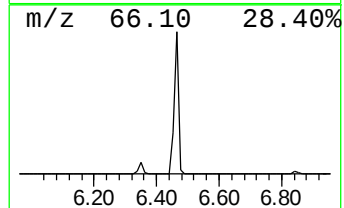
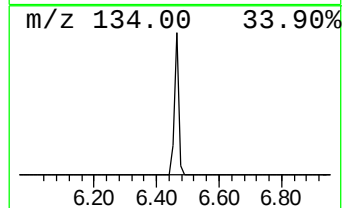
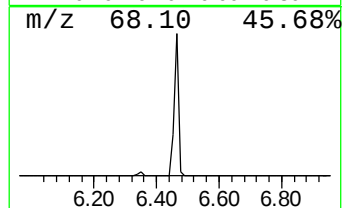
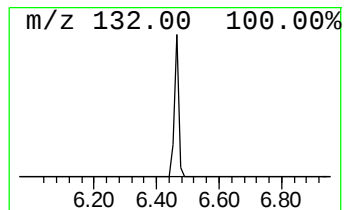
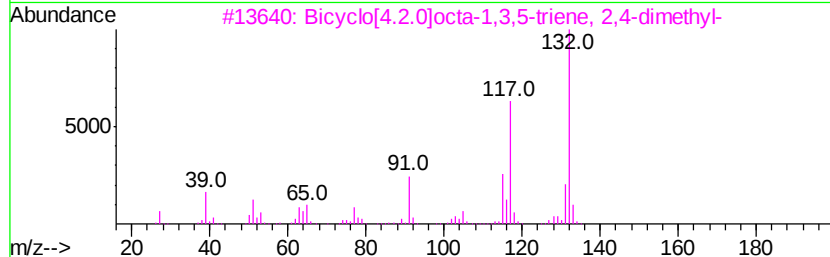
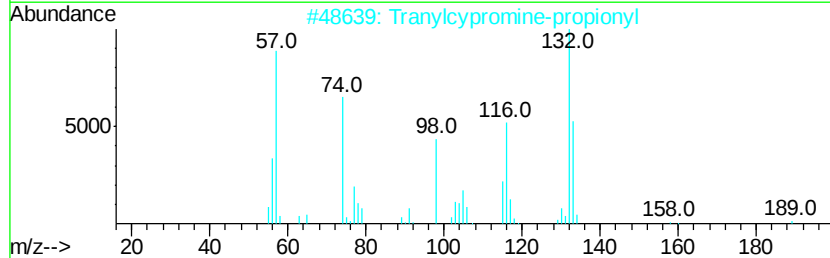
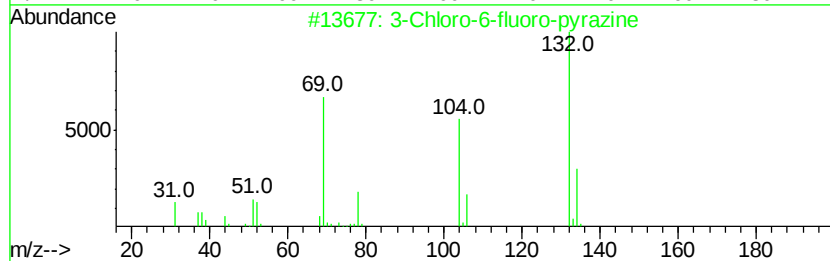
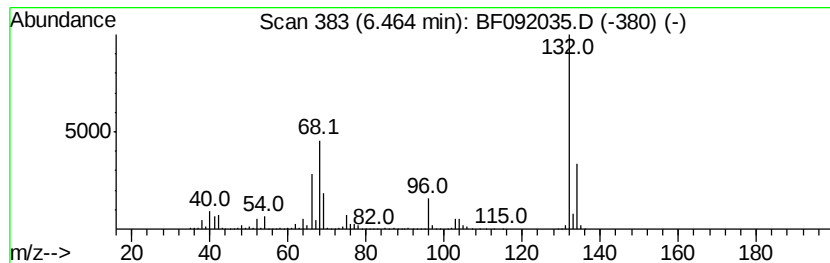
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Peak Number 2 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	84.29 ng	3864290	1,4-Dichlorobenzene-d4	6.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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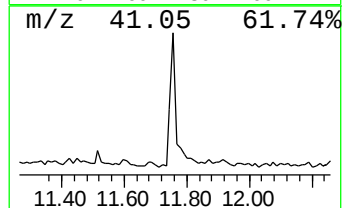
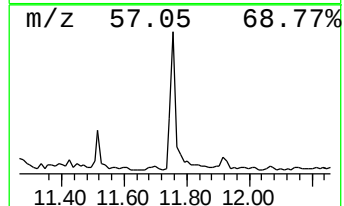
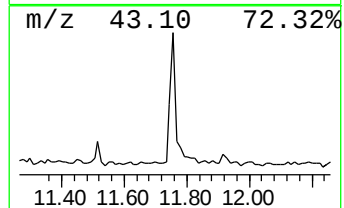
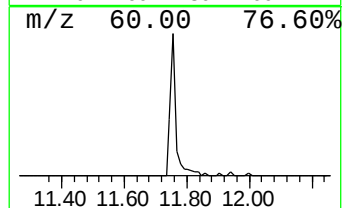
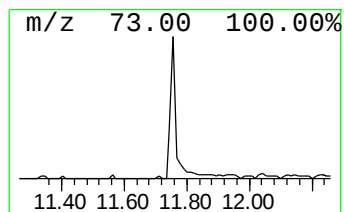
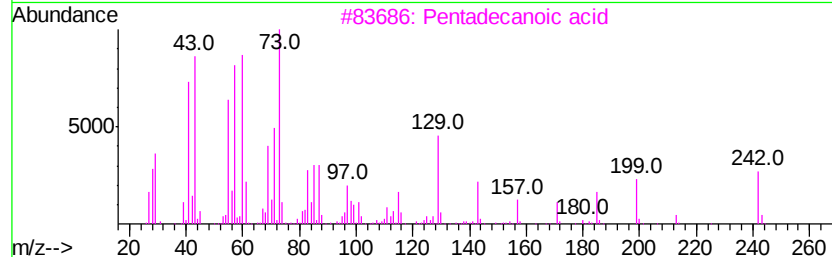
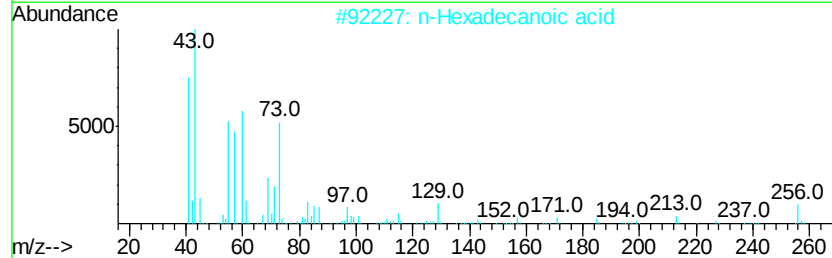
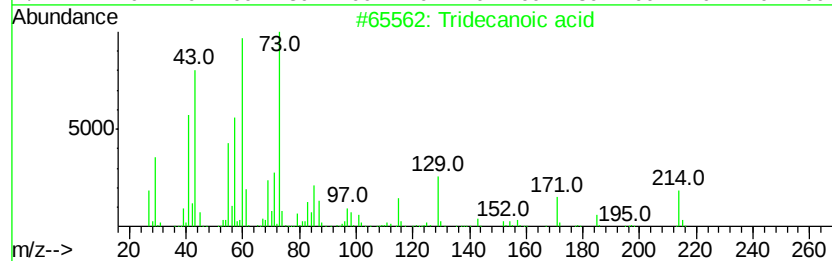
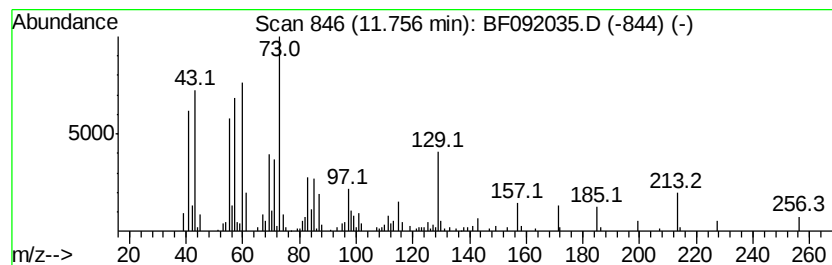
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Peak Number 4 Tridecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.76	2.89 ng	218305	Phenanthrene-d10	11.21

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	90
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	Undecanoic acid	186	C11H22O2	000112-37-8	74



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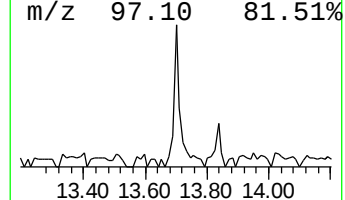
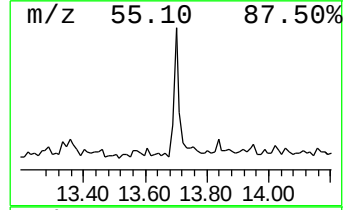
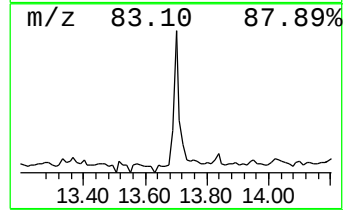
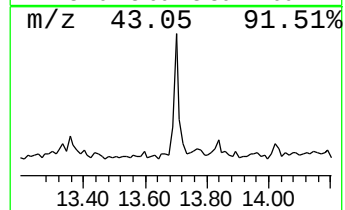
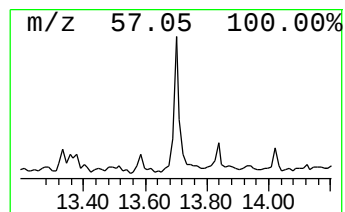
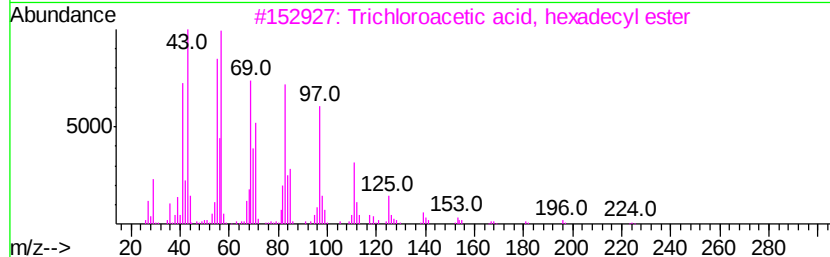
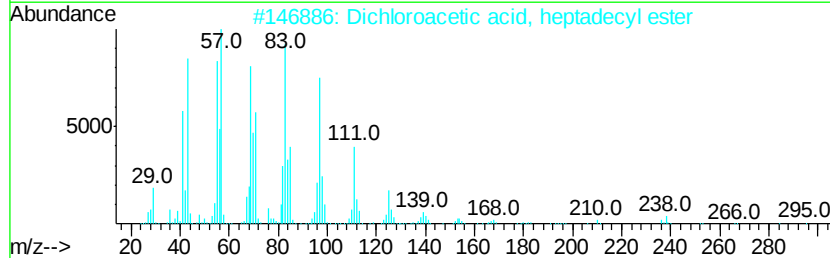
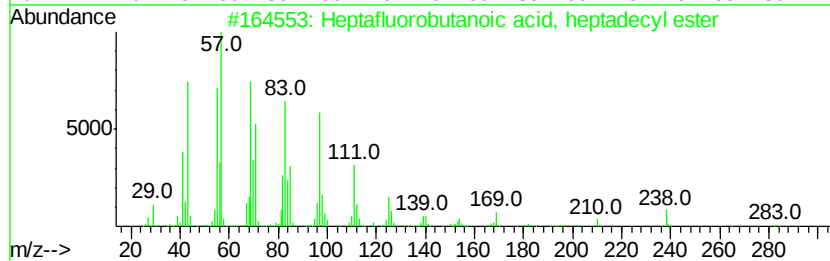
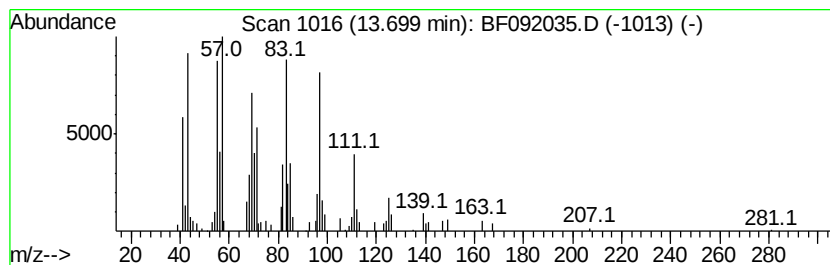
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Peak Number 6 Heptafluorobutanoic acid, h... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.70	2.09 ng	149211	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	94
2		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4		2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
5		1-Docosene	308	C22H44	001599-67-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.83	16.2	ng	743825	1	6.69	916888	20.0
unknown6.46	6.46	84.3	ng	3864290	1	6.69	916888	20.0
Tridecanoic acid	11.76	2.9	ng	218305	4	11.21	1509080	20.0
Heptafluorobutano...	13.70	2.1	ng	149211	5	13.84	1426880	20.0