

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
 Data File : BF097802.D
 Acq On : 17 Aug 2017 22:48
 Operator : SJ/JU
 Sample : I4761-04
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RUSB-04

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-BF081517.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	4.975	485	491	499	rVB	267587	361535	10.58%	1.378%
2	5.387	555	561	564	rBV	3189779	3179581	93.04%	12.119%
3	6.410	729	735	745	rBV	3305553	3417515	100.00%	13.026%
4	6.545	753	758	761	rBV	3320051	3122426	91.37%	11.901%
5	6.775	794	797	801	rVB	1085410	851368	24.91%	3.245%
6	6.934	820	824	827	rBV	2714109	2324675	68.02%	8.860%
7	7.340	888	893	896	rBV	2101469	1898097	55.54%	7.234%
8	8.057	1011	1015	1018	rBV	1258615	1009992	29.55%	3.850%
9	9.133	1193	1198	1202	rBV	2945738	2789826	81.63%	10.633%
10	9.528	1261	1265	1268	rBV	398247	302125	8.84%	1.152%
11	9.810	1309	1313	1317	rVB	1010234	860296	25.17%	3.279%
12	10.598	1442	1447	1450	rBV	1401375	1298936	38.01%	4.951%
13	10.722	1465	1468	1473	rBV	51320	52445	1.53%	0.200%
14	11.292	1561	1565	1569	rBV	882451	729119	21.33%	2.779%
15	12.880	1831	1835	1838	rBV	2304464	2063333	60.38%	7.864%
16	13.780	1983	1988	1995	rBV	197908	214094	6.26%	0.816%
17	13.927	2009	2013	2020	rVB	931720	821056	24.02%	3.129%
18	14.416	2093	2096	2102	rBV2	104624	125814	3.68%	0.480%
19	14.692	2140	2143	2145	rBV2	32902	37045	1.08%	0.141%
20	14.851	2167	2170	2173	rVB3	34725	36446	1.07%	0.139%
21	15.039	2199	2202	2204	rBV3	32428	44506	1.30%	0.170%
22	15.063	2204	2206	2212	rVB4	45678	57430	1.68%	0.219%
23	15.357	2251	2256	2260	rBV	516210	587055	17.18%	2.238%
24	15.833	2332	2337	2340	rBV4	29160	52194	1.53%	0.199%

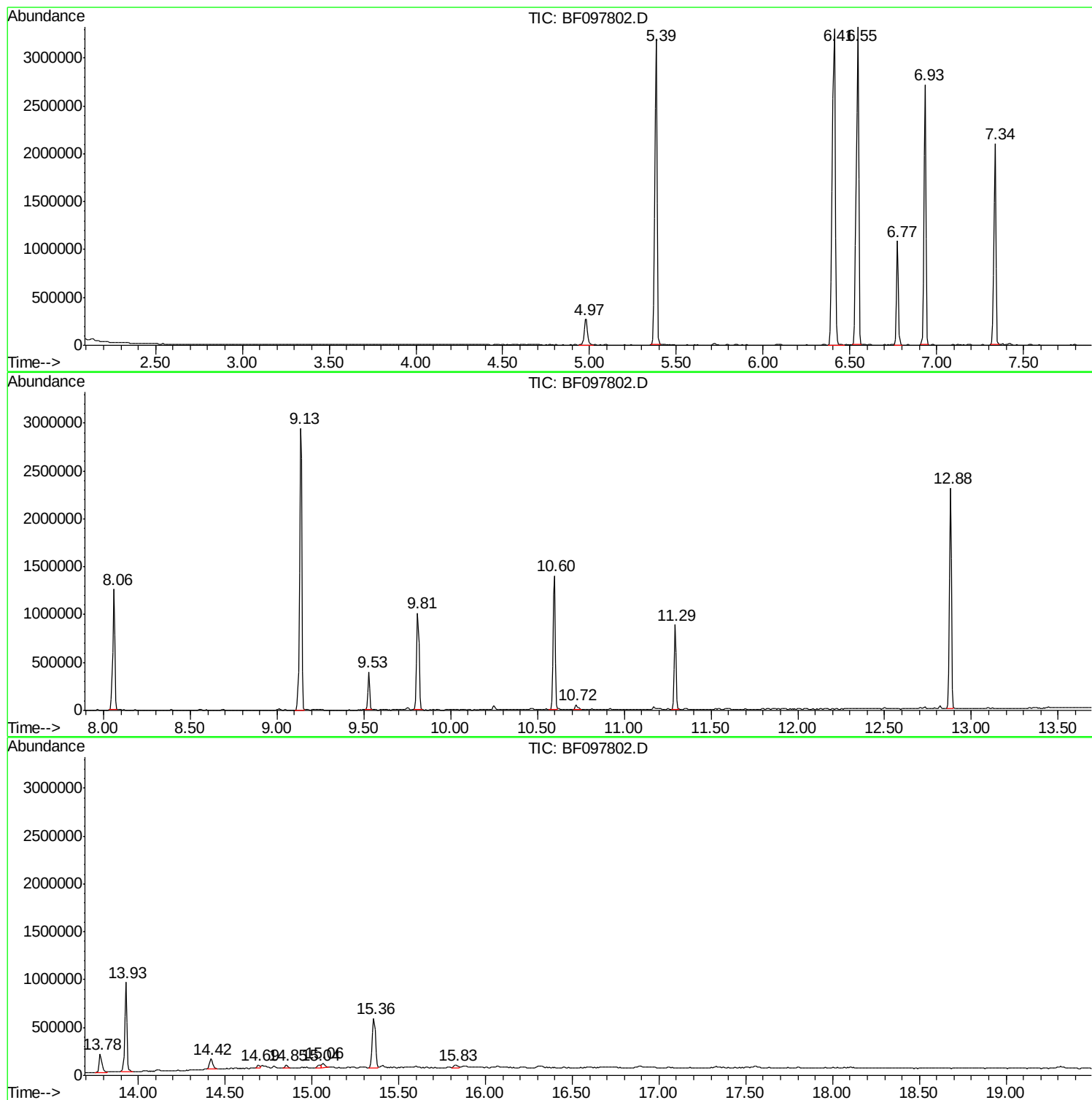
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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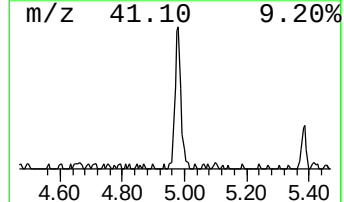
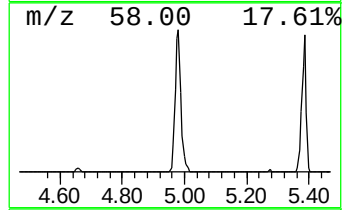
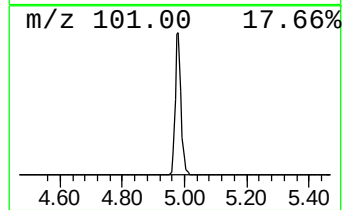
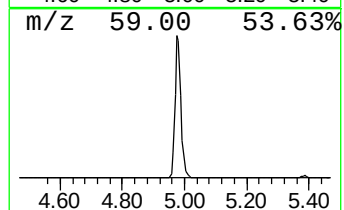
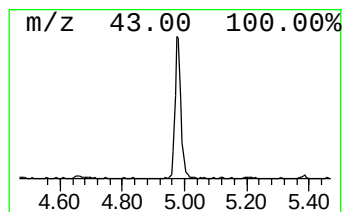
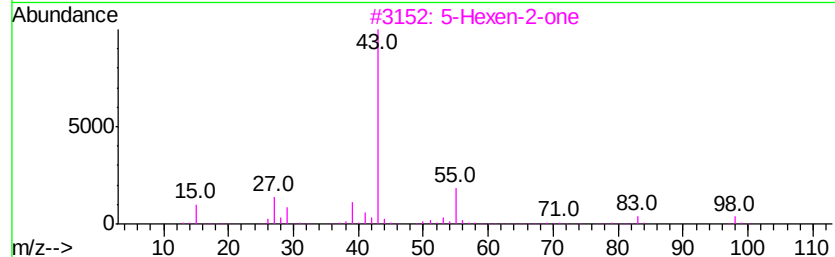
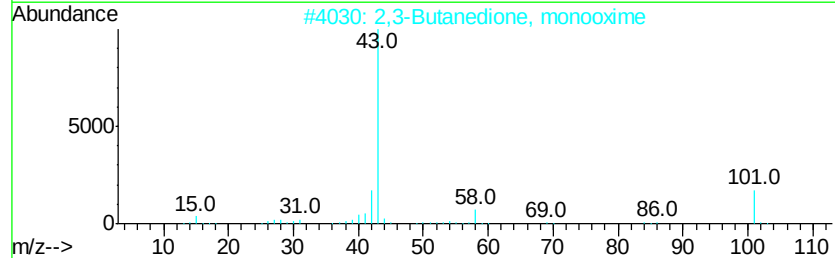
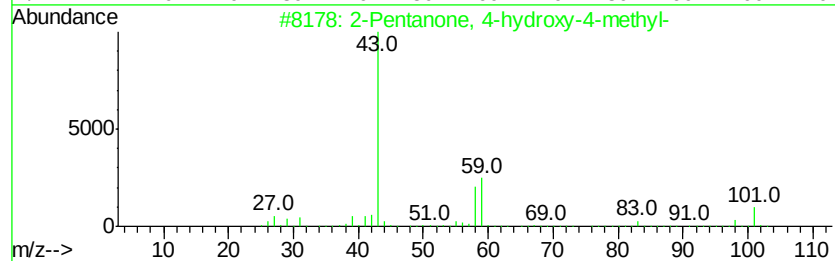
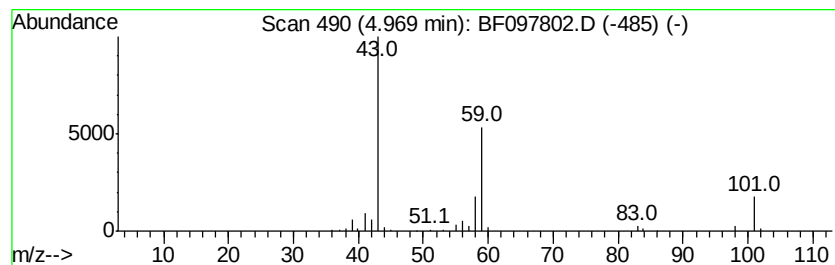
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.97	8.49 ng	361535	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
3		5-Hexen-2-one	98	C6H10O	000109-49-9	9
4		Propane, 2-methyl-2-(1-methylethyl)-	116	C7H16O	017348-59-3	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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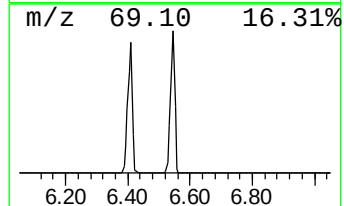
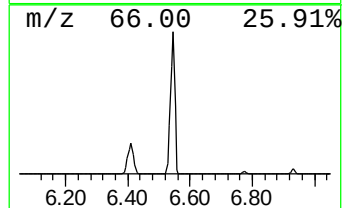
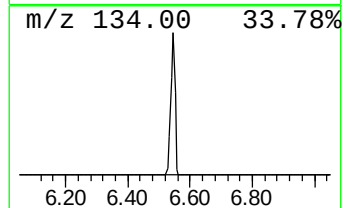
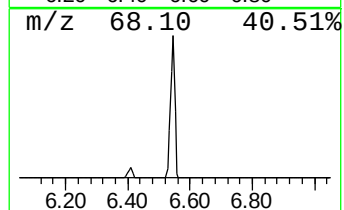
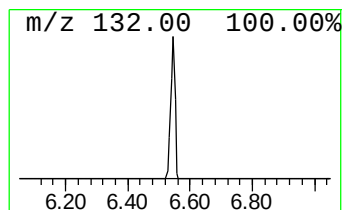
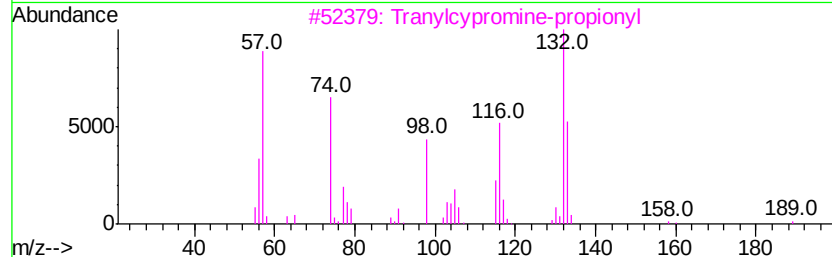
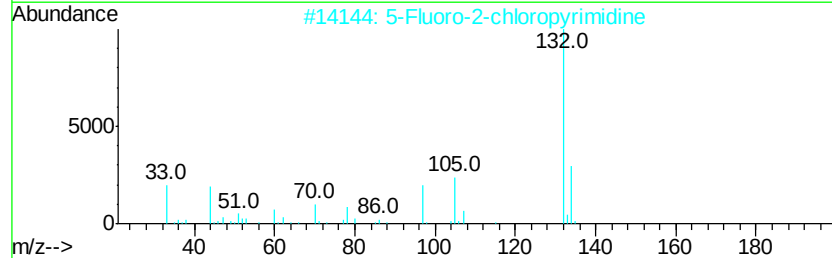
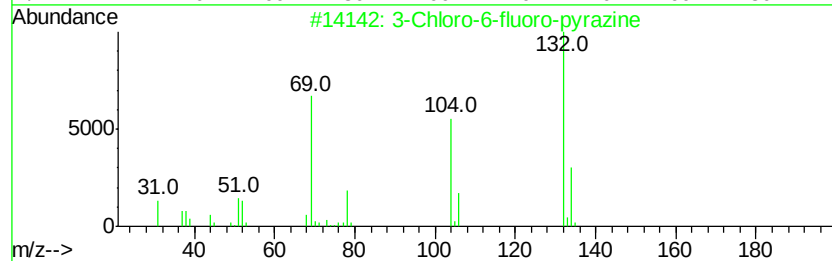
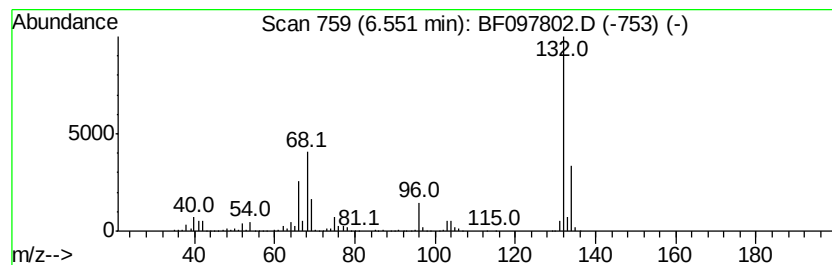
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	73.35 ng	3122430	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Xenon	132	Xe	007440-63-3	9



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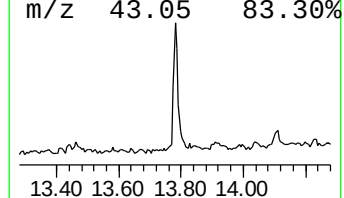
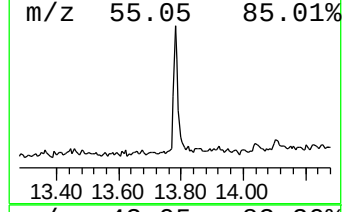
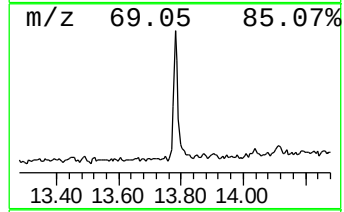
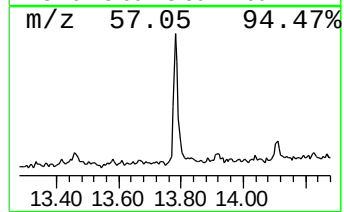
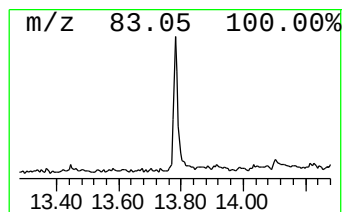
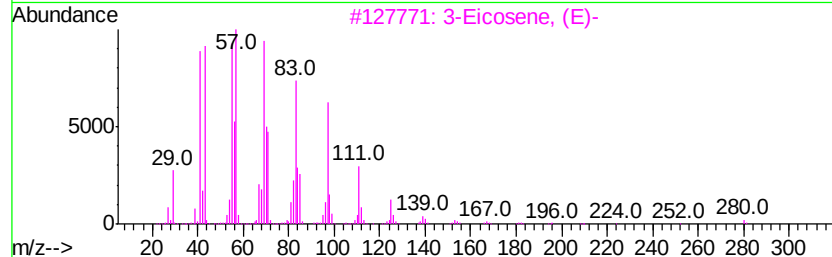
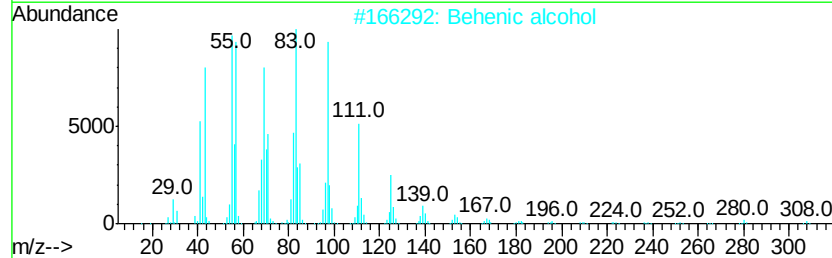
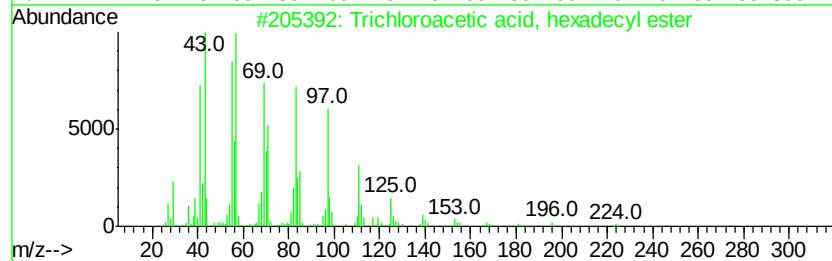
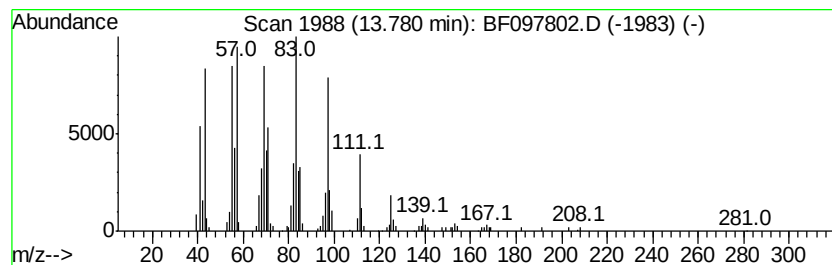
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	5.22 ng	214094	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Behenic alcohol	326	C22H46O	000661-19-8	93
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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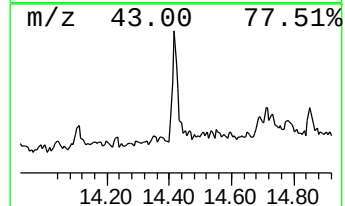
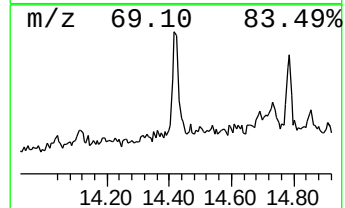
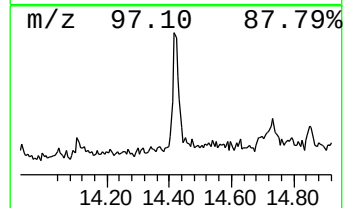
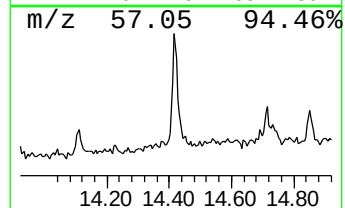
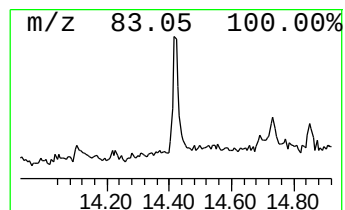
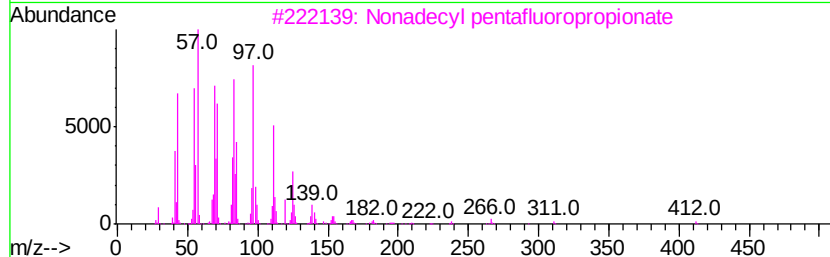
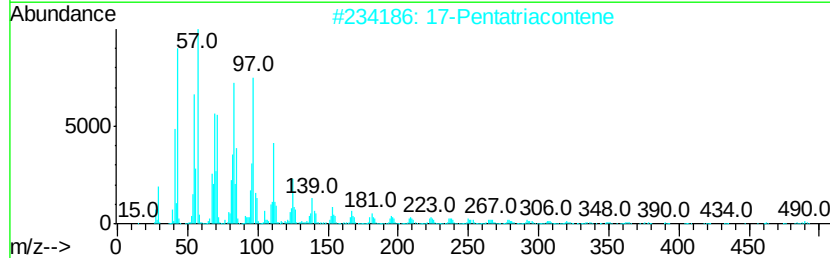
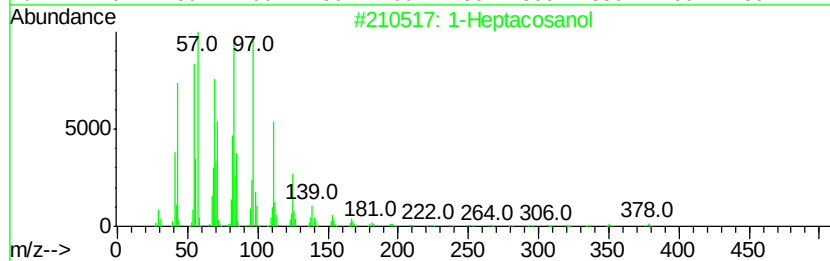
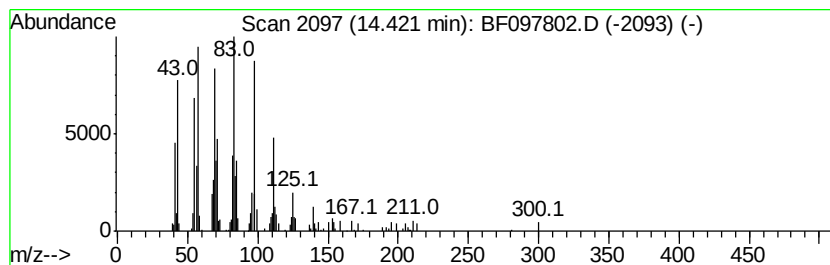
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Peak Number 5 1-Heptacosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.42	3.06 ng	125814	Chrysene-d12	13.93	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heptacosanol	396	C27H56O	002004-39-9	91
2	17-Pentatriacontene	491	C35H70	006971-40-0	91
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	90
4	1-Docosene	308	C22H44	001599-67-3	87
5	Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.97	8.5	ng	361535	1	6.77	851368	20.0
unknown6.55	6.55	73.3	ng	3122430	1	6.77	851368	20.0
Trichloroacetic a...	13.78	5.2	ng	214094	5	13.93	821056	20.0
1-Heptacosanol	14.42	3.1	ng	125814	5	13.93	821056	20.0