

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF081717\
 Data File : BF097800.D
 Acq On : 17 Aug 2017 21:51
 Operator : SJ/JU
 Sample : I4808-03
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP-TP106-K(0-5)COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 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	4.981	488	492	501	rVB	382652	525577	13.47%	1.733%
2	5.393	556	562	565	rBV	3382146	3816889	97.81%	12.585%
3	6.410	729	735	738	rBV	3515835	3902272	100.00%	12.867%
4	6.545	753	758	761	rBV	3666931	3684297	94.41%	12.148%
5	6.775	793	797	800	rBV	1069697	837064	21.45%	2.760%
6	6.934	819	824	827	rBV	3111986	2806208	71.91%	9.253%
7	7.340	887	893	896	rBV	2373022	2294548	58.80%	7.566%
8	8.057	1011	1015	1019	rBV	1240137	1017212	26.07%	3.354%
9	9.139	1193	1199	1202	rBV	3707970	3504651	89.81%	11.556%
10	9.528	1261	1265	1268	rBV	445457	350815	8.99%	1.157%
11	9.810	1308	1313	1317	rBV2	1009483	907194	23.25%	2.991%
12	10.598	1442	1447	1450	rBV	1799608	1628742	41.74%	5.370%
13	11.292	1561	1565	1569	rBV	921836	769470	19.72%	2.537%
14	12.880	1831	1835	1839	rBV	2552374	2589034	66.35%	8.537%
15	13.780	1985	1988	1995	rBV2	107931	135169	3.46%	0.446%
16	13.927	2009	2013	2016	rBV	876882	772445	19.79%	2.547%
17	14.692	2139	2143	2151	rBV2	134611	200552	5.14%	0.661%
18	15.357	2251	2256	2260	rBV	496543	586316	15.02%	1.933%

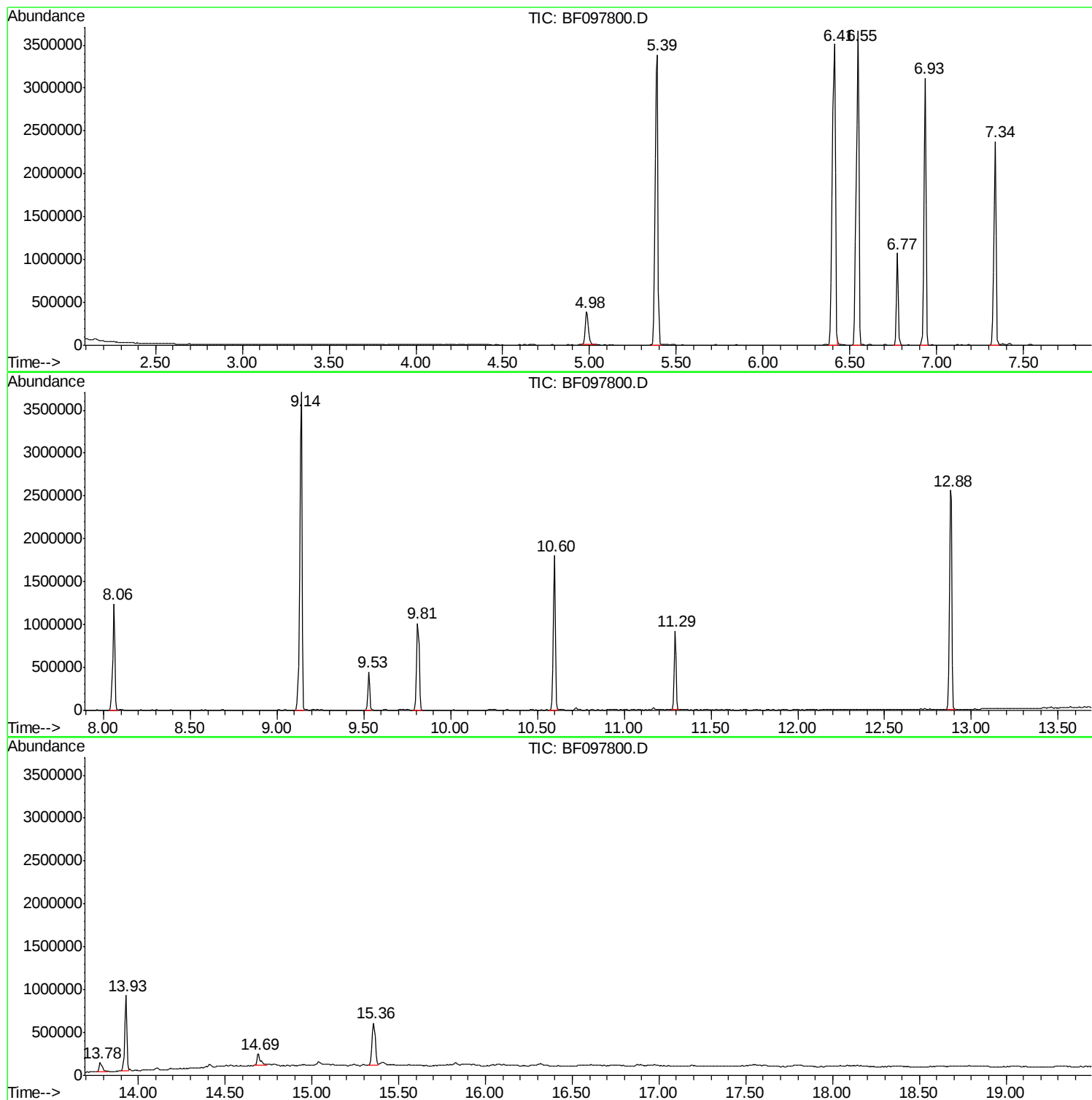
Sum of corrected areas: 30328455

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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



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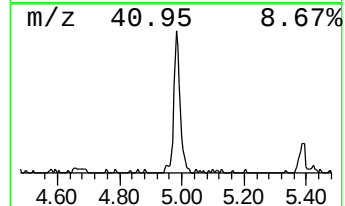
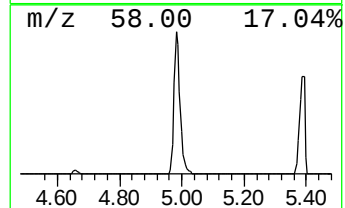
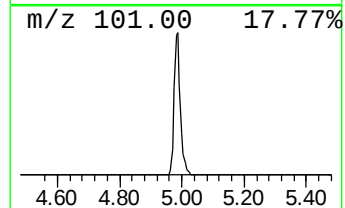
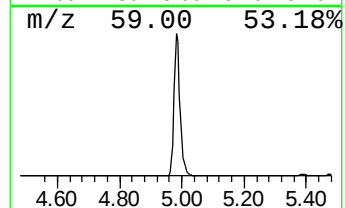
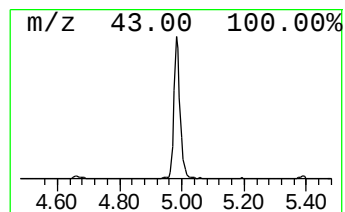
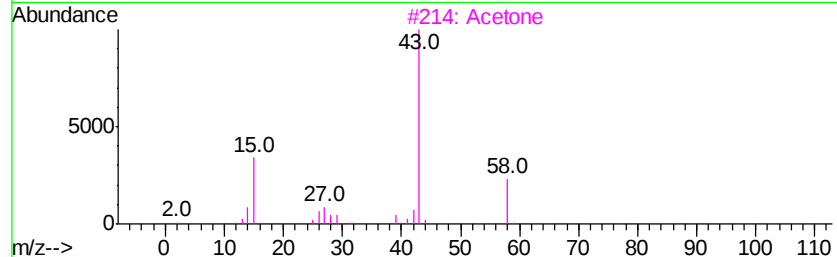
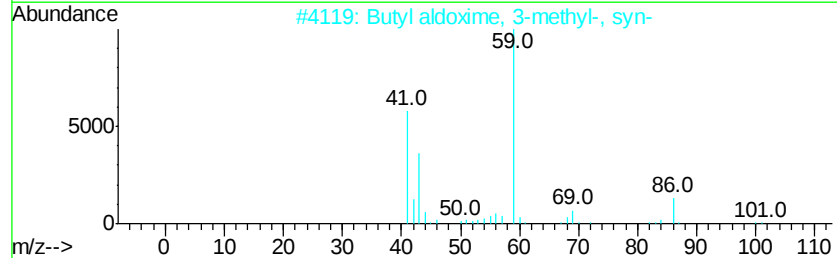
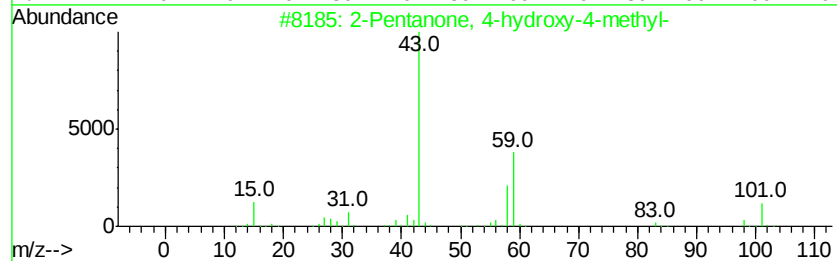
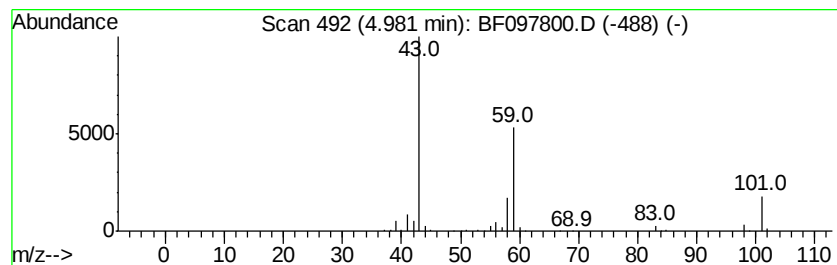
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.98	12.56 ng	525577	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	59
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3		Acetone	58	C3H6O	000067-64-1	12
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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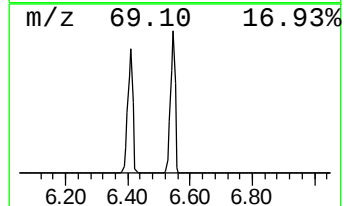
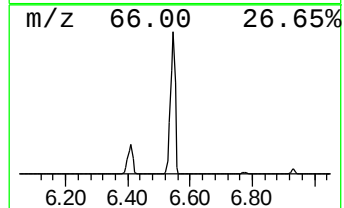
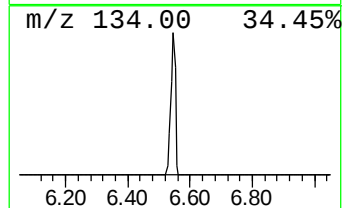
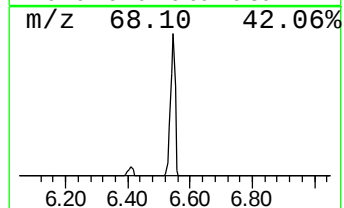
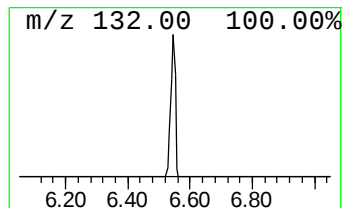
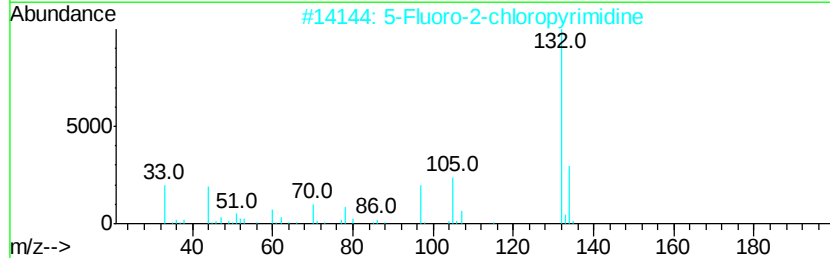
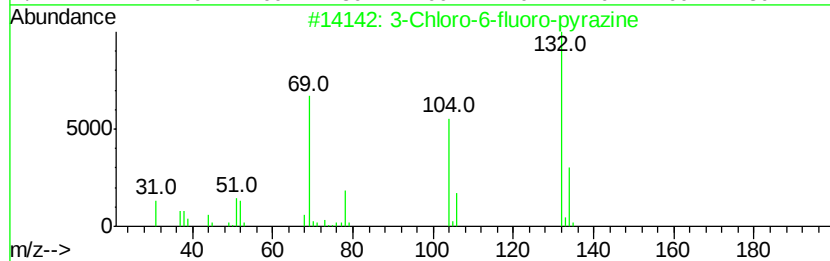
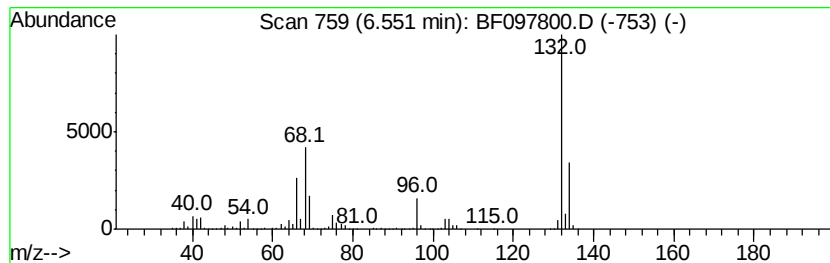
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Peak Number 2 unknown6.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.55	88.03 ng	3684300	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		Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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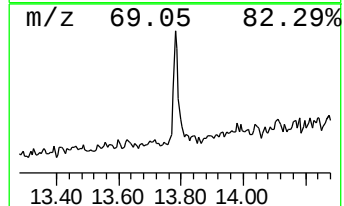
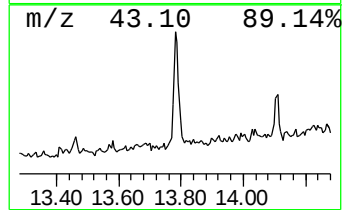
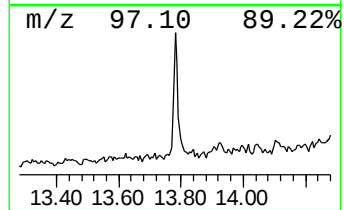
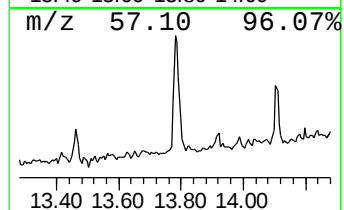
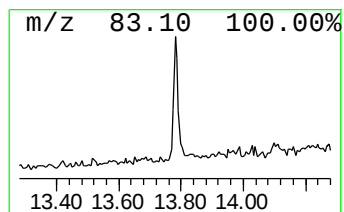
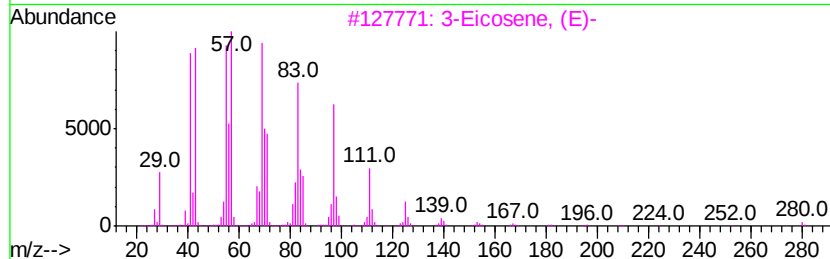
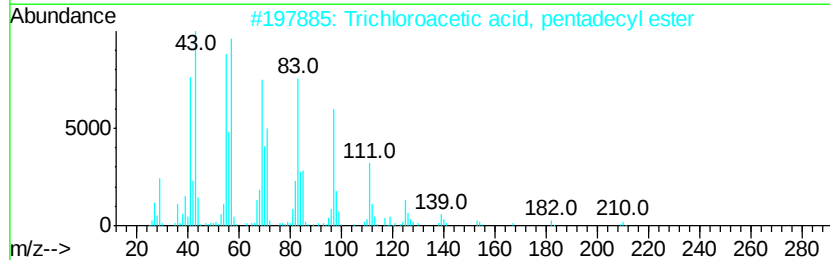
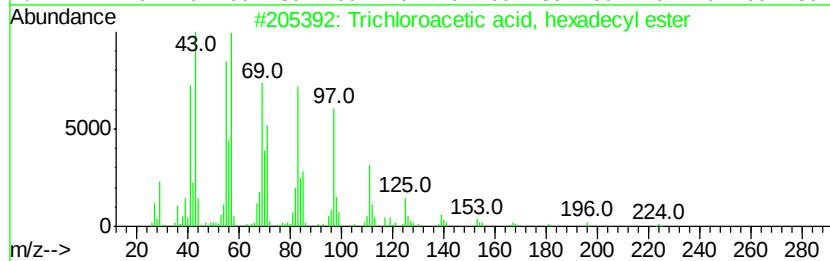
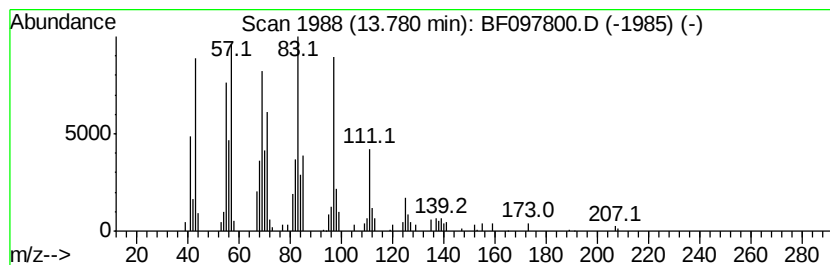
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Peak Number 4 Trichloroacetic acid, hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	3.50 ng	135169	Chrysene-d12	13.93

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		3-Eicosene, (E)-	280	C20H40	074685-33-9	91
4		11-Tricosene	322	C23H46	052078-56-5	90
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	87



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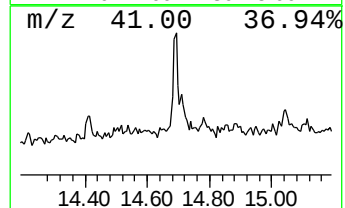
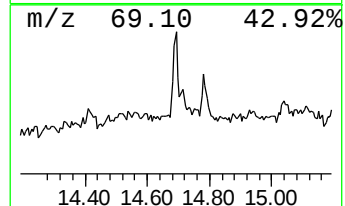
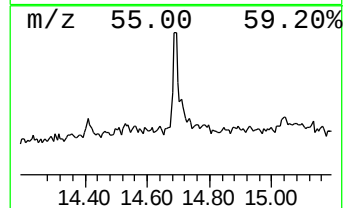
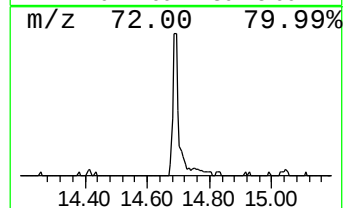
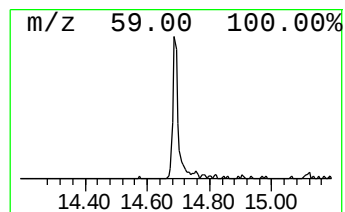
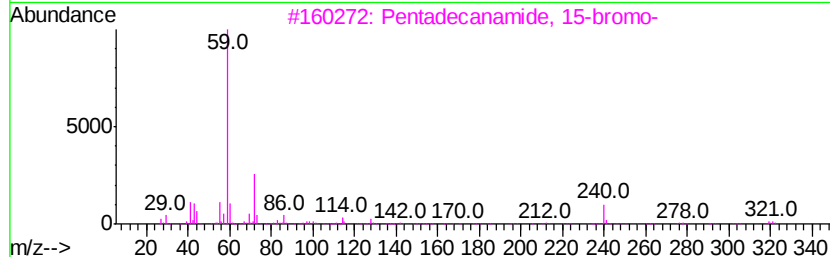
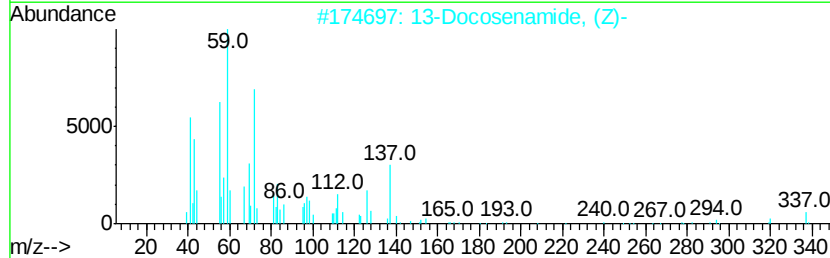
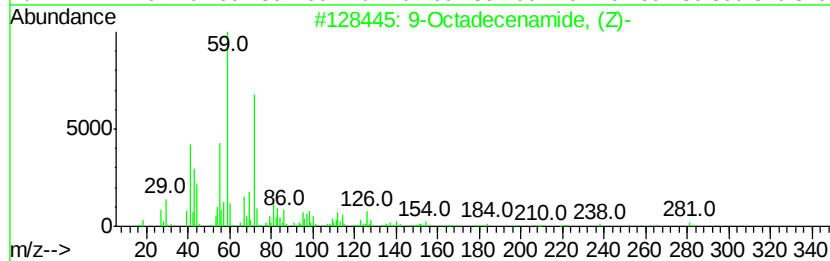
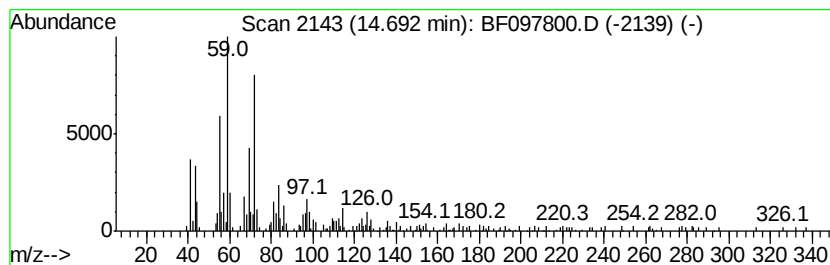
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	6.84 ng	200552	Perylene-d12	15.36

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	87
2		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	83
3		Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	50
4		Octadecanamide	283	C18H37NO	000124-26-5	43
5		Tetradecanamide	227	C14H29NO	000638-58-4	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.98	12.6	ng	525577	1	6.77	837064	20.0
unknown6.55	6.55	88.0	ng	3684300	1	6.77	837064	20.0
Trichloroacetic a...	13.78	3.5	ng	135169	5	13.93	772445	20.0
9-Octadecenamide,...	14.69	6.8	ng	200552	6	15.36	586316	20.0