

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100715\
 Data File : BF082117.D
 Acq On : 7 Oct 2015 21:35
 Operator : UM/IZ
 Sample : G3924-01
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MGP213BR-50-51

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-BF092815.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	5.051	252	255	267	rVB	695472	1059994	35.60%	4.810%
2	5.463	289	291	294	rBV	1406299	2064402	69.34%	9.367%
3	6.503	379	382	385	rBV	1712474	1911997	64.22%	8.676%
4	6.640	391	394	396	rBV	2300246	2215334	74.41%	10.052%
5	6.869	412	414	426	rVB	352881	433762	14.57%	1.968%
6	7.029	426	428	430	rBV	1802106	1618835	54.37%	7.346%
7	7.440	461	464	470	rBV	1196616	1270164	42.66%	5.764%
8	7.520	470	471	478	rVB	20768	47871	1.61%	0.217%
9	8.160	525	527	533	rBV2	642339	714983	24.01%	3.244%
10	9.235	619	621	624	rBV	2174881	2129206	71.52%	9.662%
11	9.635	653	656	658	rBV	457963	418043	14.04%	1.897%
12	9.920	678	681	683	rBV	492051	690181	23.18%	3.132%
13	10.709	747	750	752	rBV	1618423	1713959	57.57%	7.777%
14	10.812	758	759	764	rVB	48393	62401	2.10%	0.283%
15	11.258	797	798	804	rBV2	28947	48399	1.63%	0.220%
16	11.406	809	811	813	rBV	605984	689723	23.17%	3.130%
17	11.932	854	857	859	rBV	104066	110681	3.72%	0.502%
18	12.709	923	925	930	rBV2	19589	30572	1.03%	0.139%
19	12.995	947	950	952	rBV	2822108	2977251	100.00%	13.510%
20	13.887	1025	1028	1037	rBV	99338	205719	6.91%	0.933%
21	14.047	1039	1042	1053	rVB	610988	786742	26.43%	3.570%
22	14.790	1105	1107	1112	rBV2	69556	106041	3.56%	0.481%
23	14.881	1112	1115	1117	rVB	50182	55120	1.85%	0.250%
24	15.487	1165	1168	1182	rBV	456155	676665	22.73%	3.070%

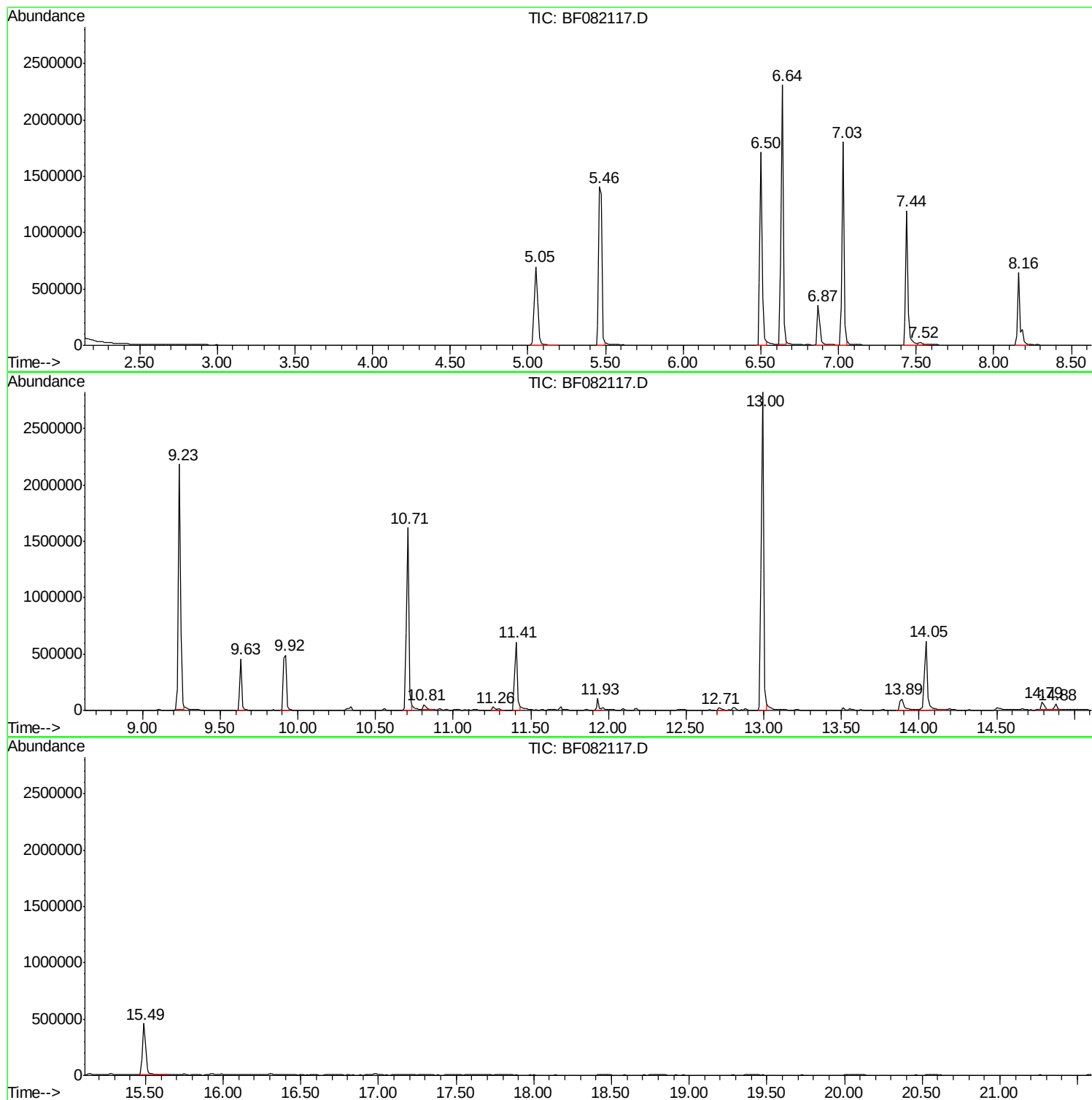
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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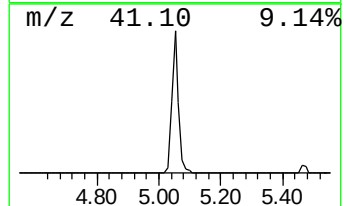
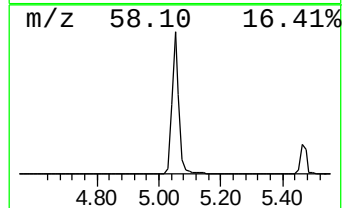
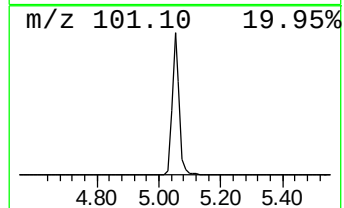
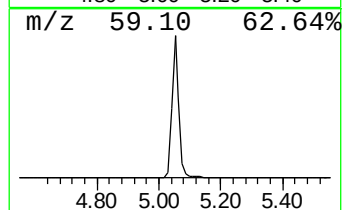
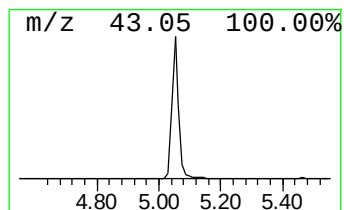
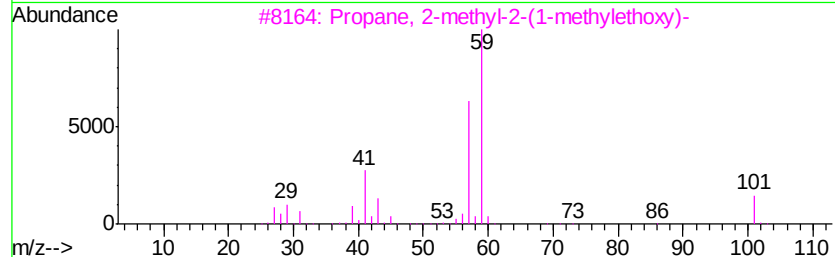
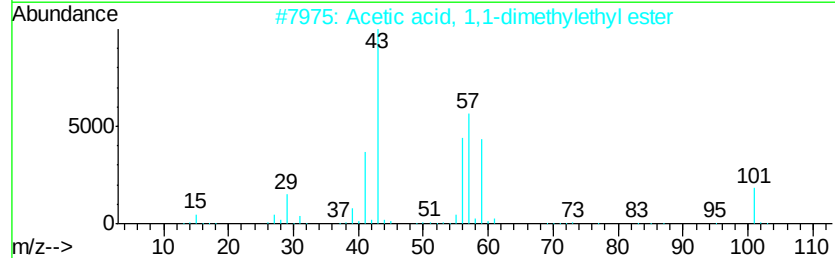
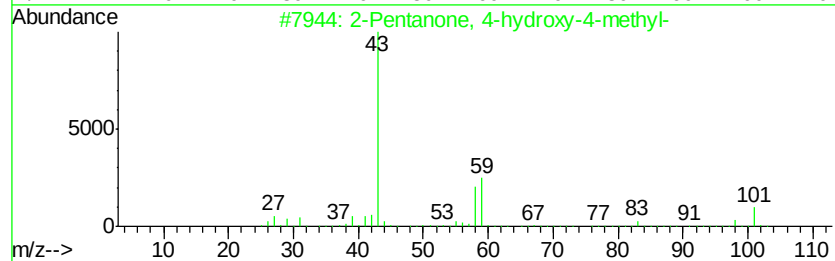
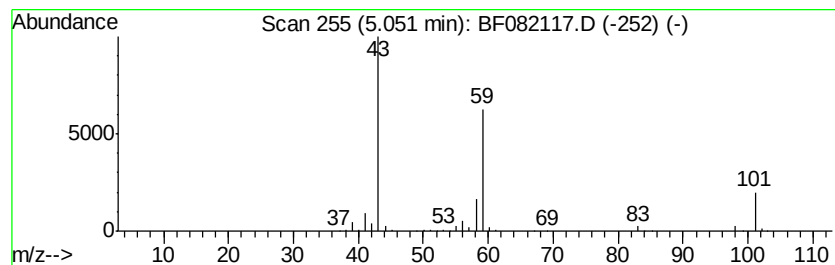
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092815.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.05	48.87 ng	1059990	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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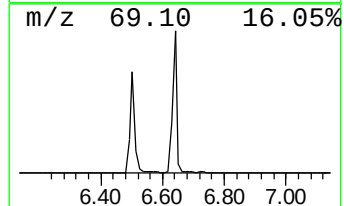
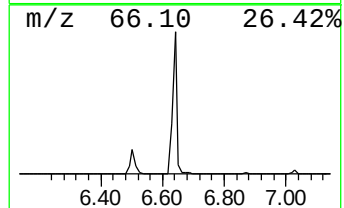
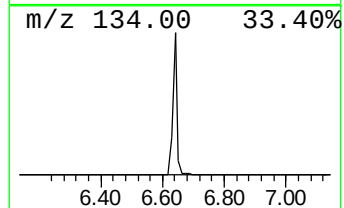
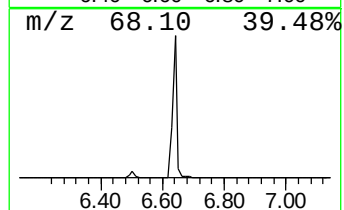
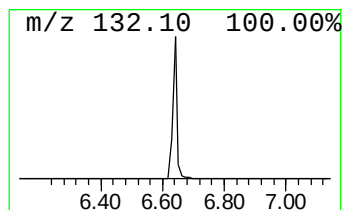
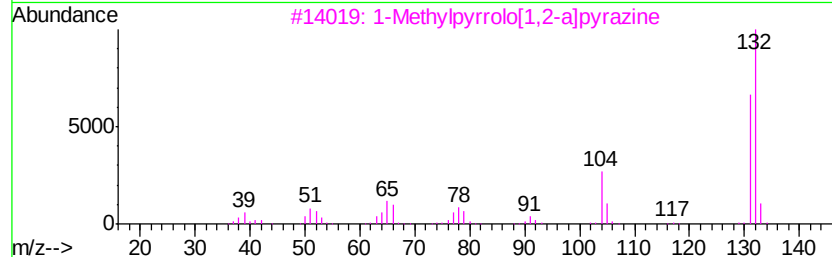
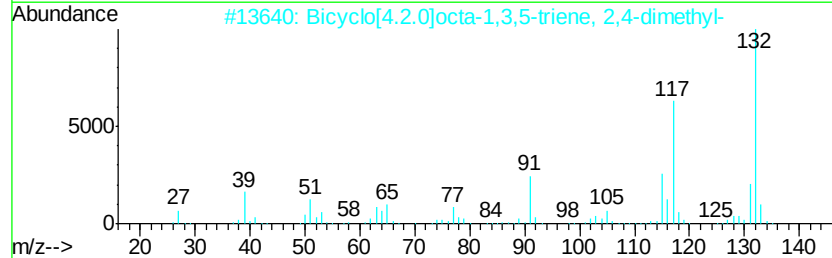
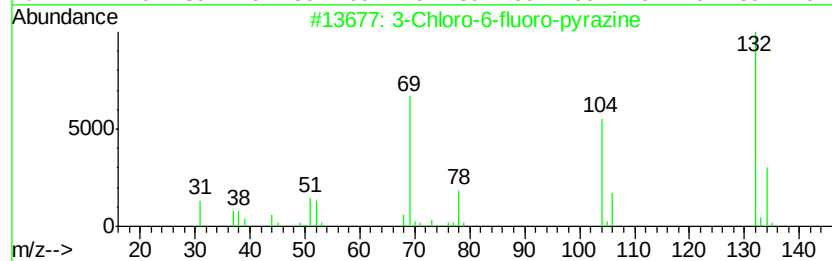
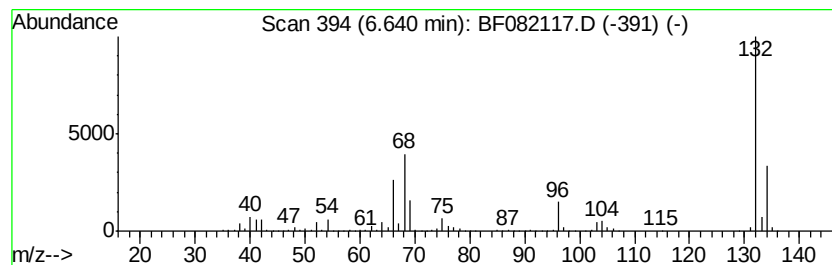
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.64	102.15 ng	2215330	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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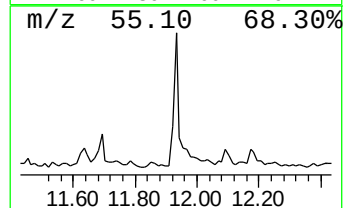
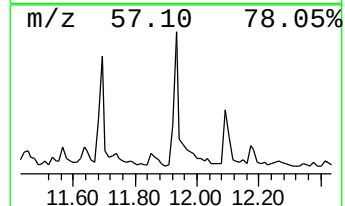
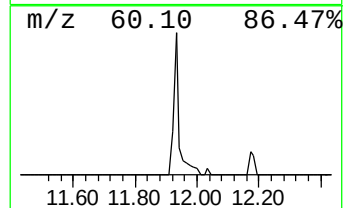
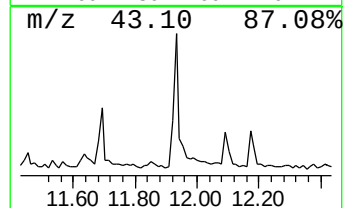
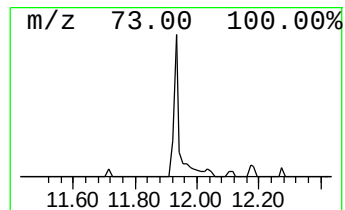
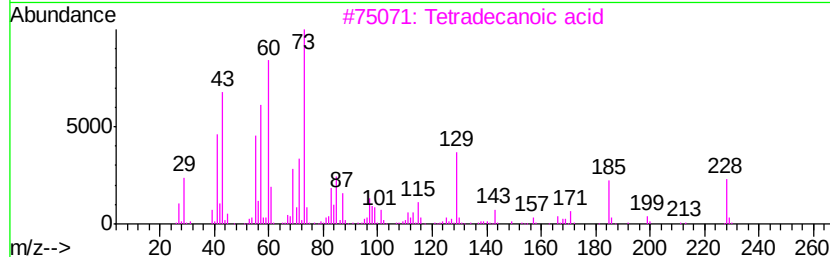
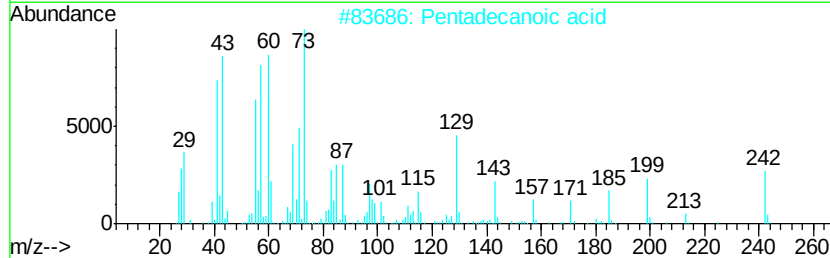
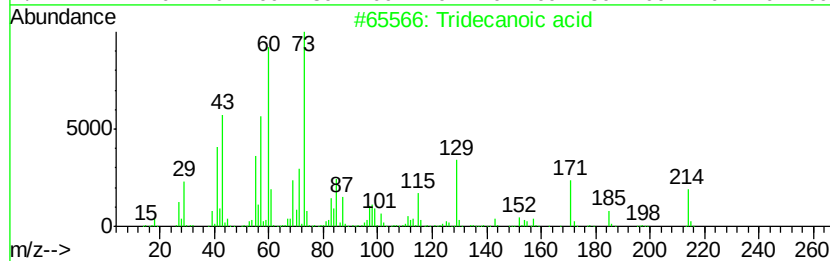
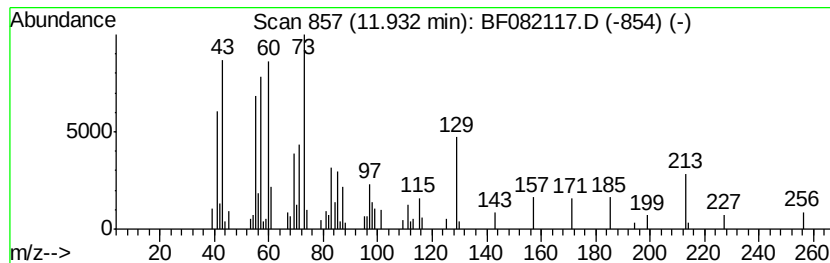
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Peak Number 4 Tridecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.93	3.21 ng	110681	Phenanthrene-d10	11.41

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Tridecanoic acid	214	C13H26O2	000638-53-9	90
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4		Ethanol, 2-(hexadecyloxy)-	286	C18H38O2	002136-71-2	14
5		Dodecane	170	C12H26	000112-40-3	11



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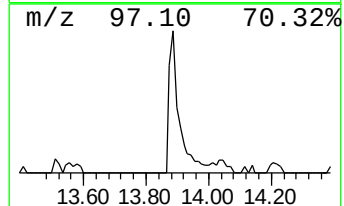
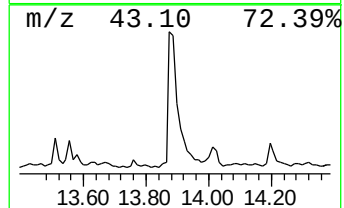
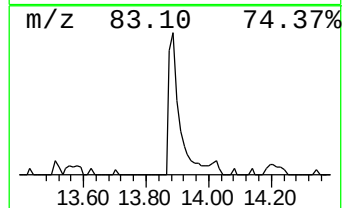
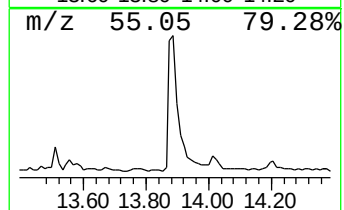
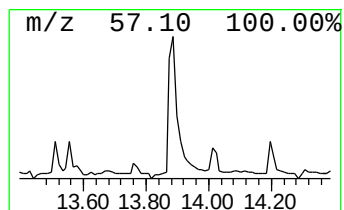
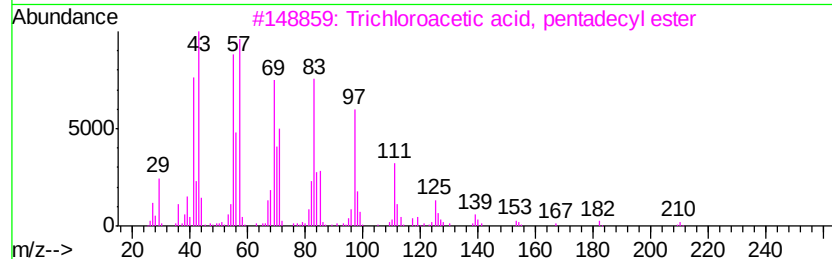
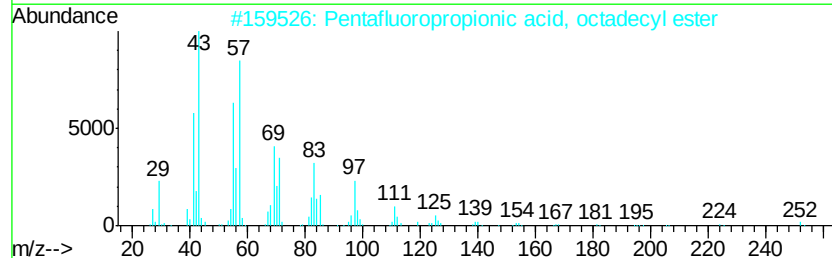
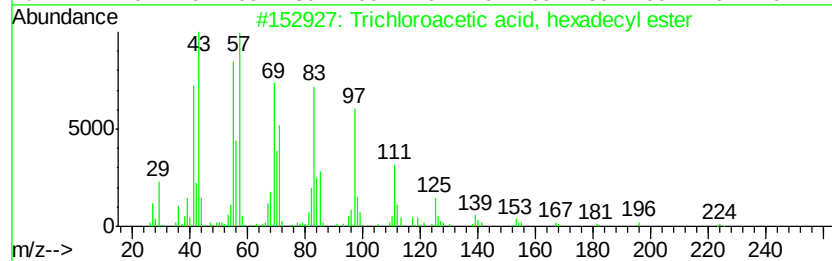
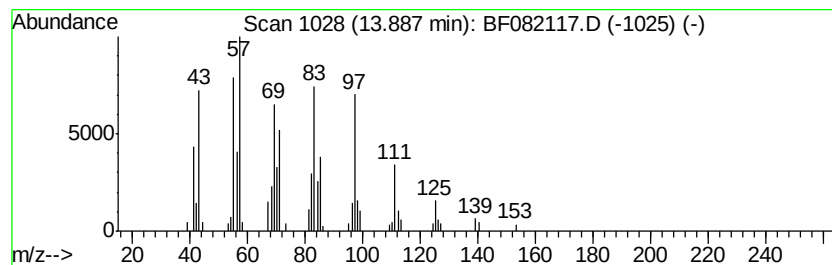
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Peak Number 5 Trichloroacetic acid, hexad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.89	5.23 ng	205719	Chrysene-d12	14.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
2		Pentafluoropropionic acid, octad...	416	C21H37F5O2	1000280-07-7	91
3		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4		1-Docosene	308	C22H44	001599-67-3	90
5		17-Pentatriacontene	491	C35H70	006971-40-0	87



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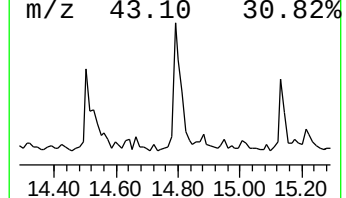
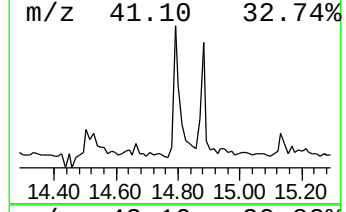
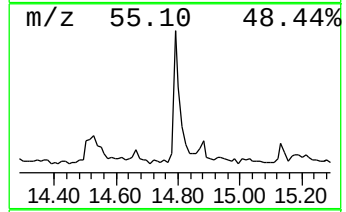
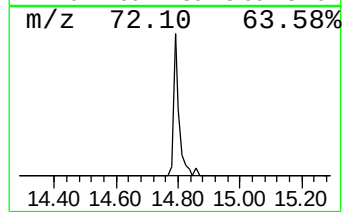
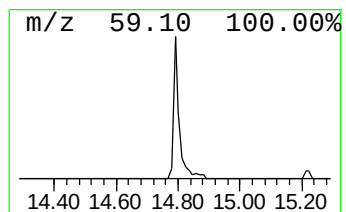
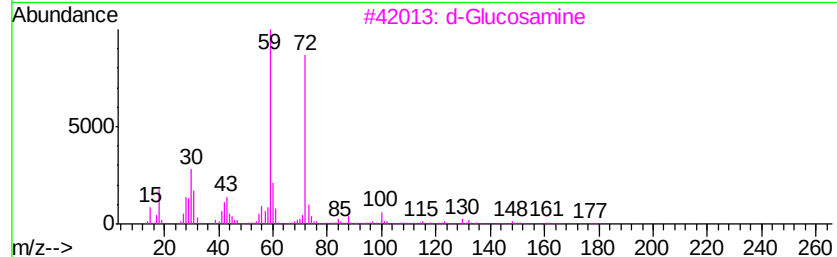
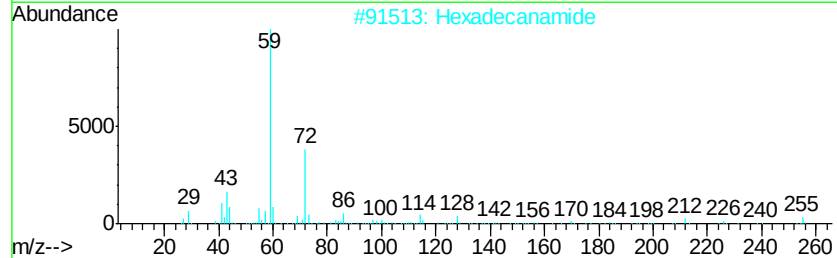
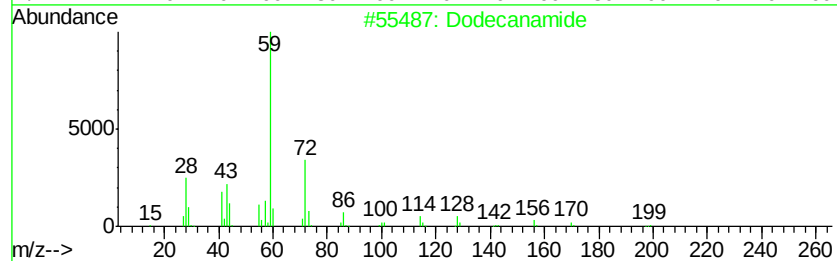
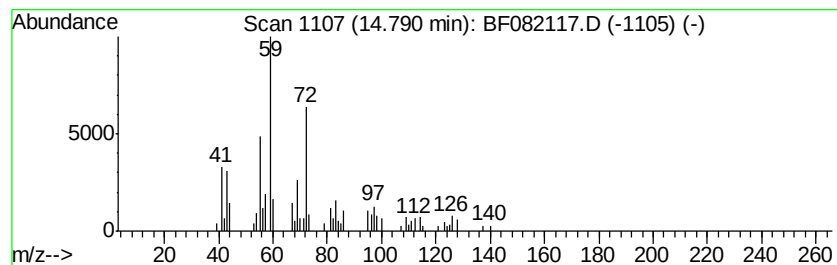
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Peak Number 6 Dodecanamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.79	3.13 ng	106041	Perylene-d12	15.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecanamide	199	C12H25NO	001120-16-7	53
2		Hexadecanamide	255	C16H33NO	000629-54-9	50
3		d-Glucosamine	179	C6H13NO5	000090-77-7	42
4		9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	38
5		2-Furanmethanol, 5-ethenyltetrahydrofuran-2-ylidene...	170	C10H18O2	005989-33-3	37



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.05	48.9	ng	1059990	1	6.87	433762	20.0
unknown6.64	6.64	102.2	ng	2215330	1	6.87	433762	20.0
Tridecanoic acid	11.93	3.2	ng	110681	4	11.41	689723	20.0
Trichloroacetic a...	13.89	5.2	ng	205719	5	14.05	786742	20.0
Dodecanamide	14.79	3.1	ng	106041	6	15.49	676665	20.0