

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF042916\
 Data File : BF086490.D
 Acq On : 29 Apr 2016 14:18
 Operator : UM/SJ
 Sample : H2704-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TEC-MW1

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-BF042716.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	4.270	188	191	194	rBV	1944422	2520414	47.01%	6.316%
2	4.944	246	250	253	rBV	2225036	3642104	67.93%	9.128%
3	5.367	284	287	289	rBV	1168140	1332747	24.86%	3.340%
4	5.778	320	323	325	rBV	474189	630198	11.75%	1.579%
5	6.407	375	378	380	rBV	670802	795863	14.84%	1.995%
6	6.544	387	390	392	rBV	1791734	2516362	46.94%	6.306%
7	6.773	408	410	415	rBV	1059605	1062222	19.81%	2.662%
8	6.933	421	424	426	rBV	3650914	3660443	68.28%	9.174%
9	7.344	456	460	462	rBV	2823582	3233243	60.31%	8.103%
10	8.064	520	523	525	rBV	1119076	1309947	24.43%	3.283%
11	9.139	614	617	620	rBV	4013412	5042240	94.05%	12.636%
12	9.539	649	652	654	rBV	74401	97398	1.82%	0.244%
13	9.813	673	676	678	rBV	1717681	1591667	29.69%	3.989%
14	10.247	711	714	716	rBV3	48662	95556	1.78%	0.239%
15	10.476	730	734	737	rBV	29768	58702	1.09%	0.147%
16	10.602	742	745	747	rBV	2185250	2419002	45.12%	6.062%
17	10.727	754	756	763	rVB	94958	136136	2.54%	0.341%
18	11.173	793	795	796	rBV	62841	58361	1.09%	0.146%
19	11.299	803	806	808	rBV	1023239	1466004	27.34%	3.674%
20	12.705	927	929	931	rBV	73234	82752	1.54%	0.207%
21	12.888	942	945	947	rBV	4217509	5361320	100.00%	13.436%
22	13.459	989	995	997	rBV	63210	79714	1.49%	0.200%
23	13.779	1021	1023	1033	rBV	81040	147722	2.76%	0.370%
24	13.928	1033	1036	1038	rBV	1004368	1363700	25.44%	3.418%
25	15.322	1155	1158	1166	rBV	857219	1198392	22.35%	3.003%

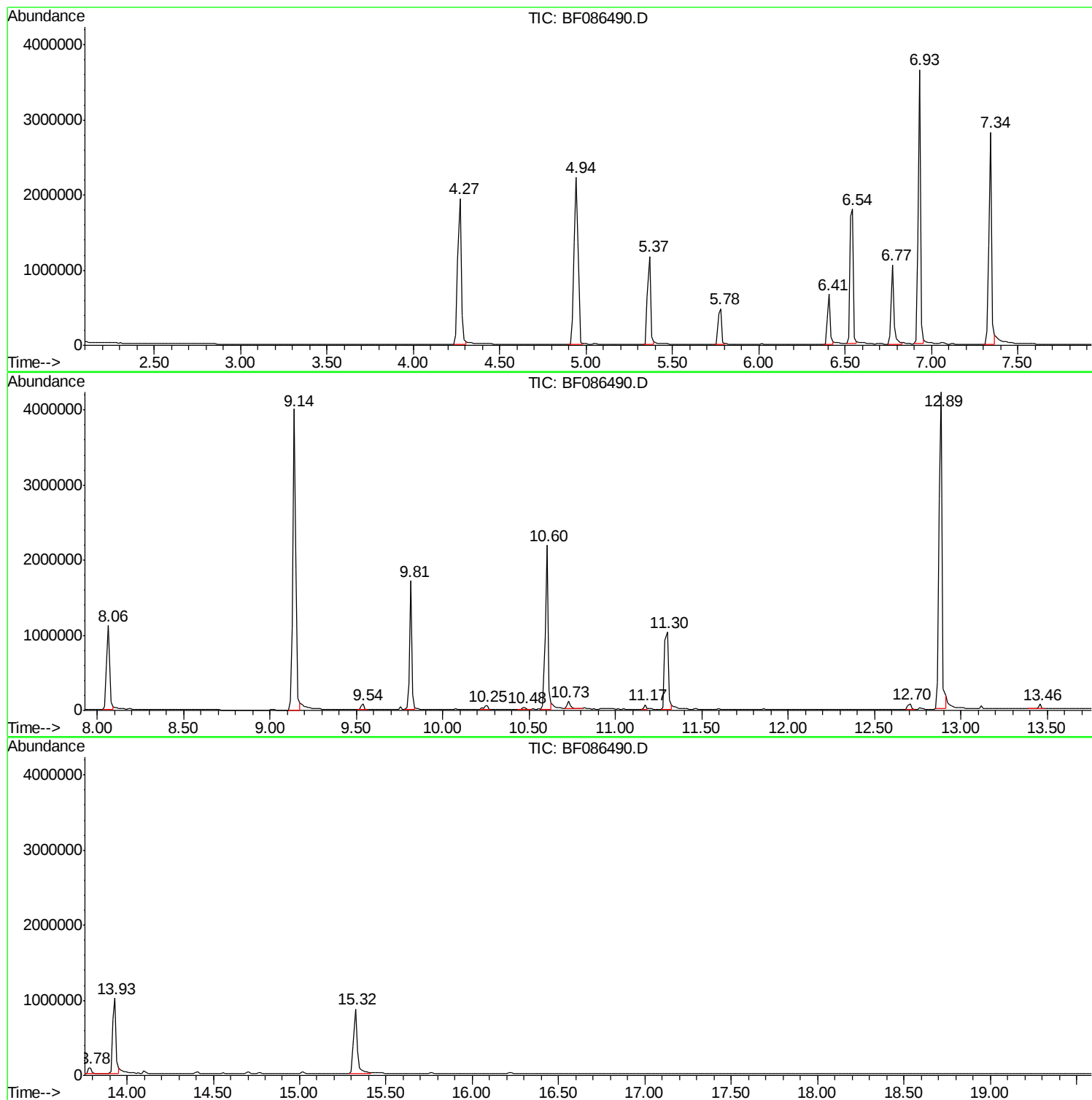
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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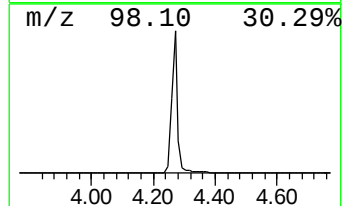
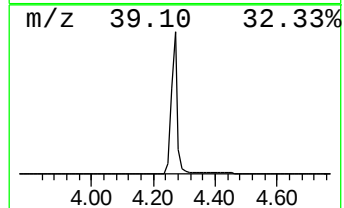
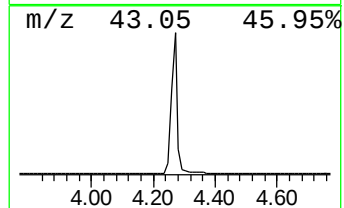
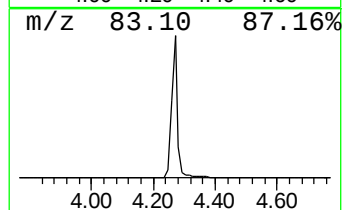
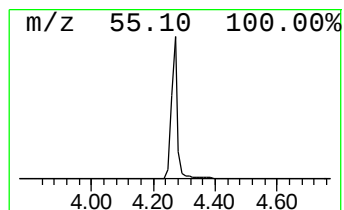
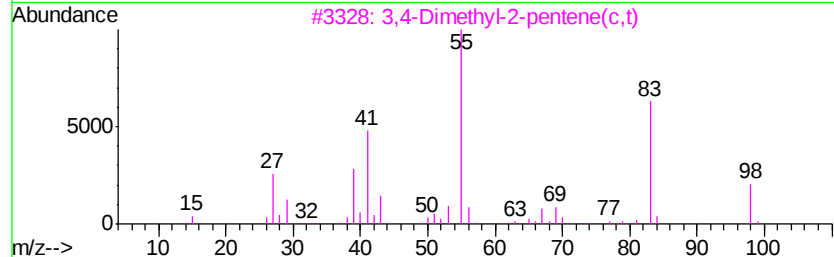
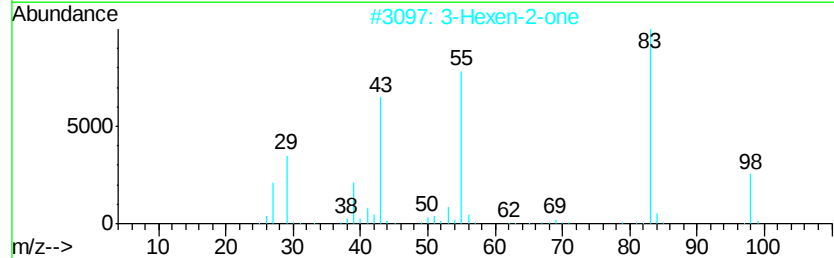
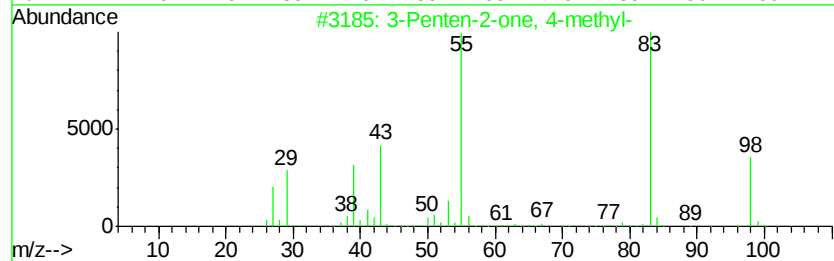
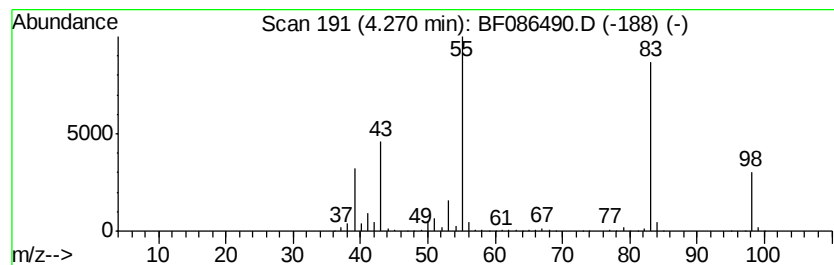
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF042716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.27	47.46 ng	2520410	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86



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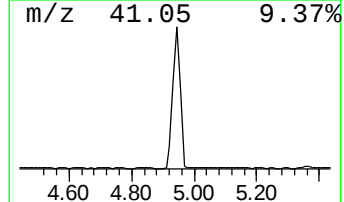
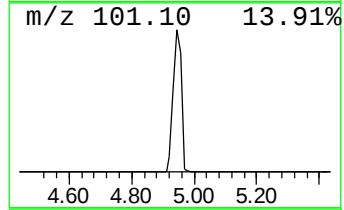
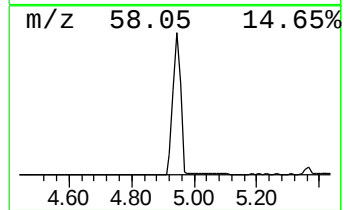
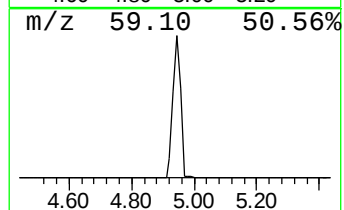
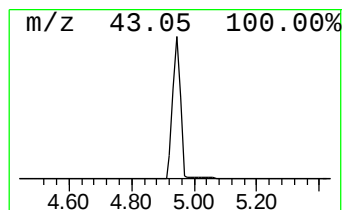
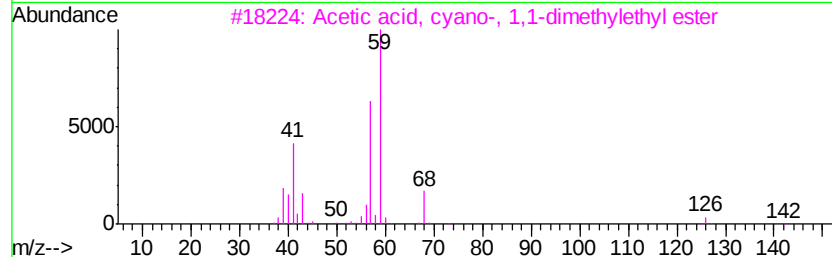
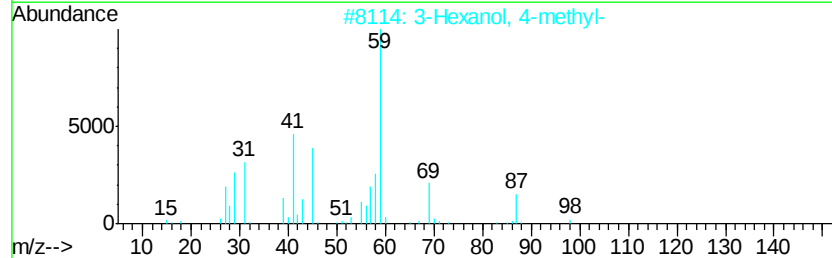
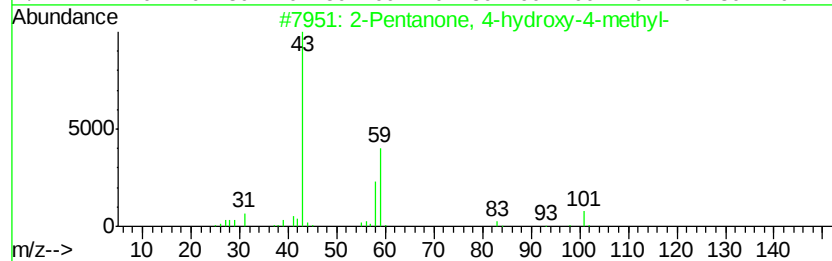
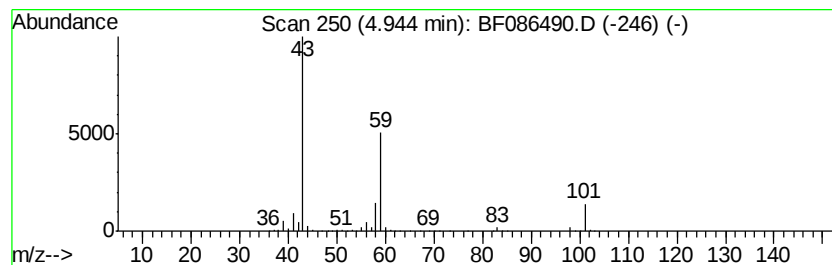
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.94	68.58 ng	3642100	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	50
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
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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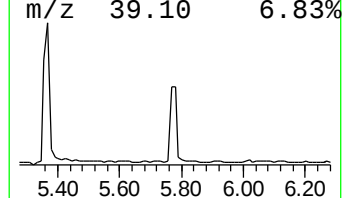
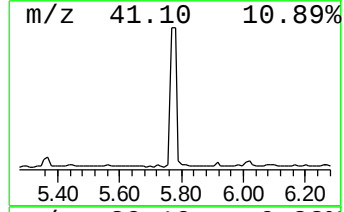
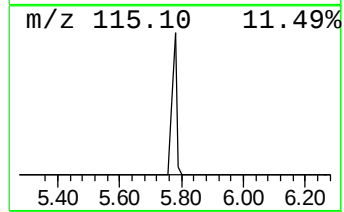
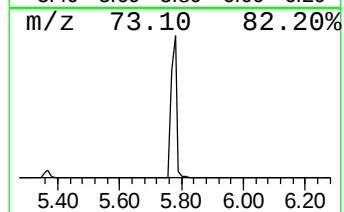
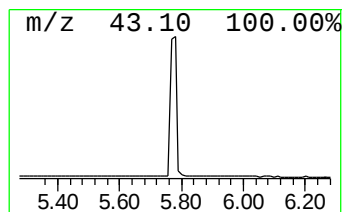
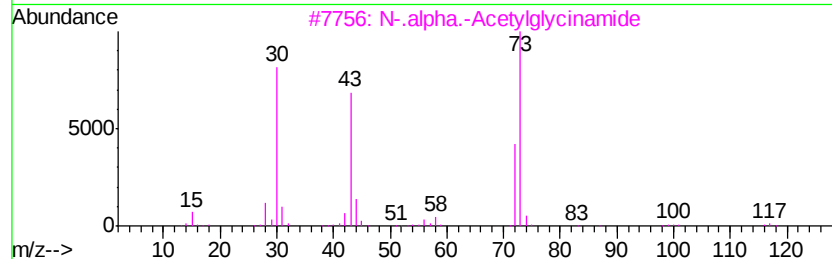
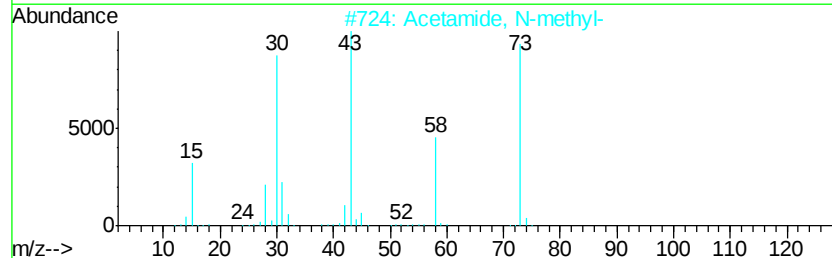
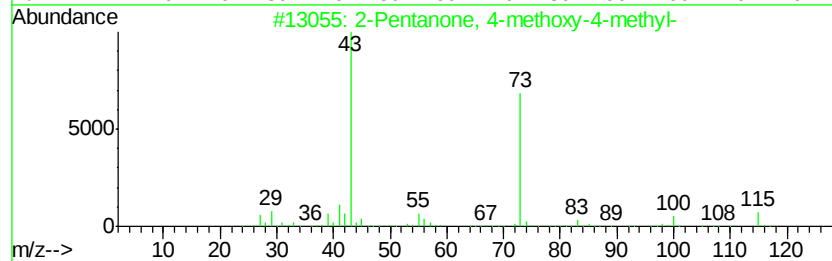
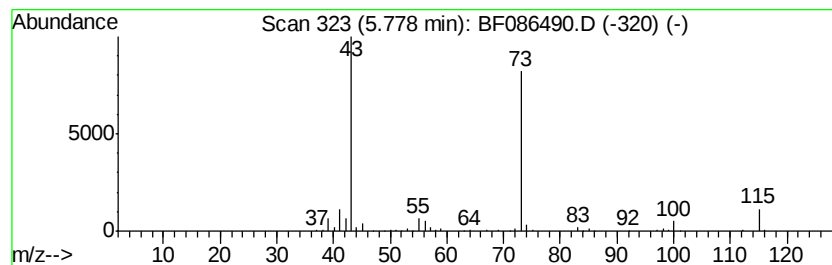
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TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-methoxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.78	11.87 ng	630198	1,4-Dichlorobenzene-d4	6.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3		N-.alpha.-Acetylglucineamide	116	C4H8N2O2	002620-63-5	25
4		2-Pentanone, 3-methyl-	100	C6H12O	000565-61-7	9
5		N-Formylmorpholine	115	C5H9NO2	004394-85-8	9



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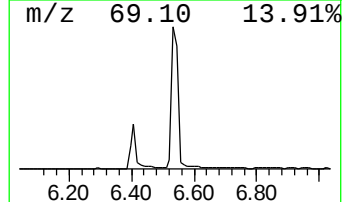
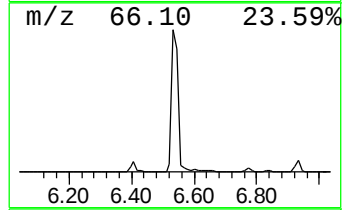
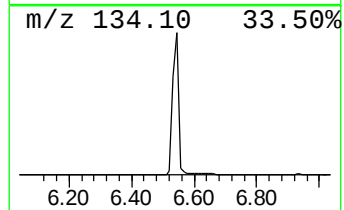
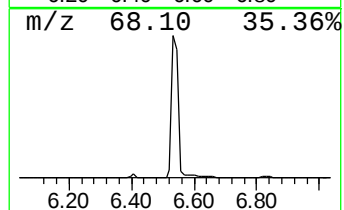
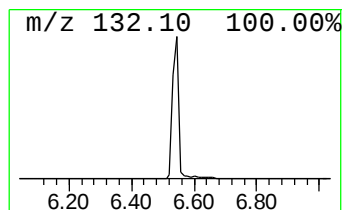
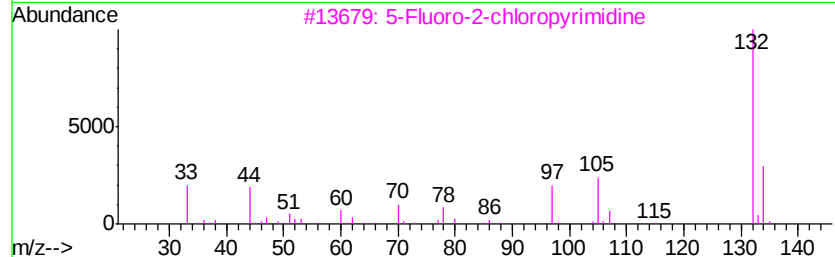
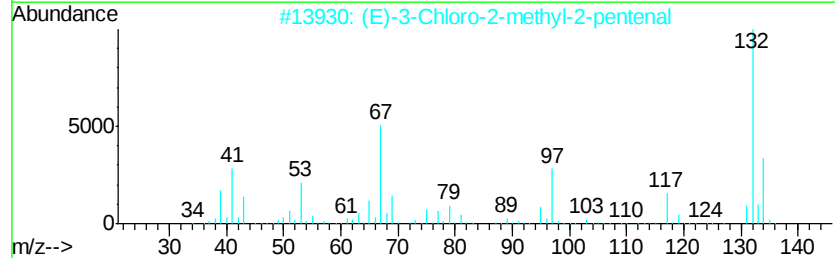
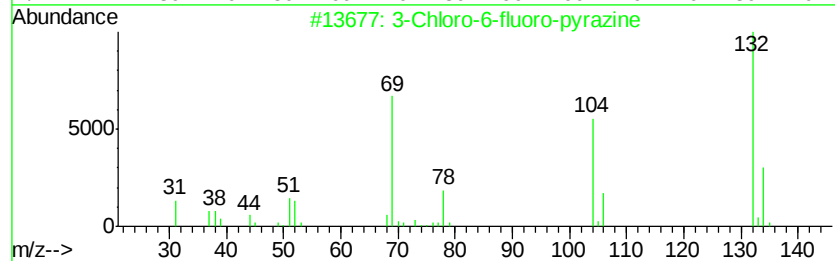
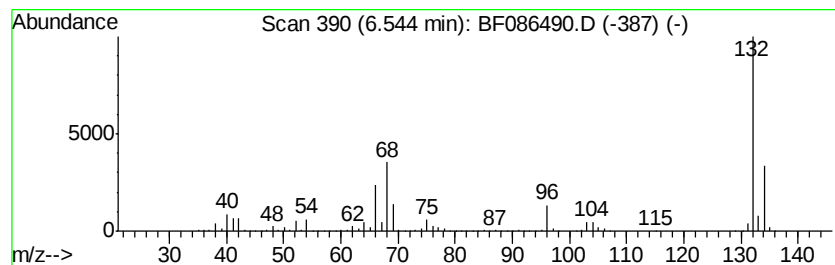
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Peak Number 4 unknown6.54 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.54	47.38 ng	2516360	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	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	16
5		5-Aminoindole	132	C8H8N2	005192-03-0	16



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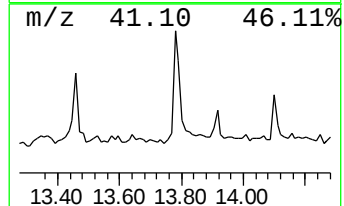
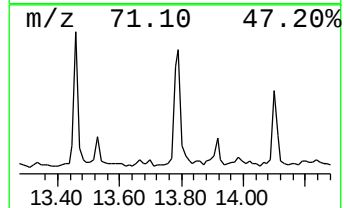
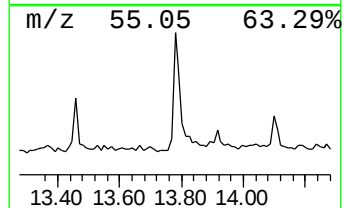
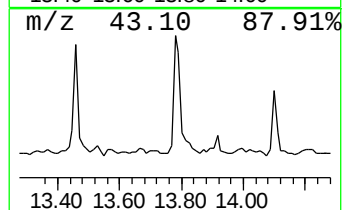
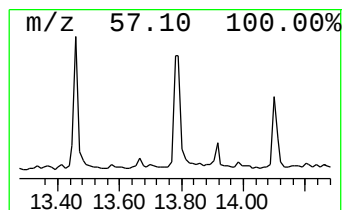
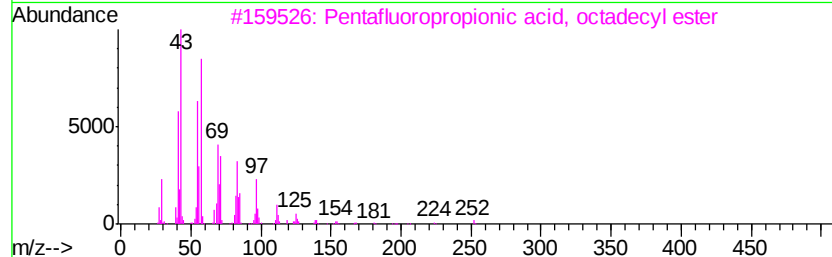
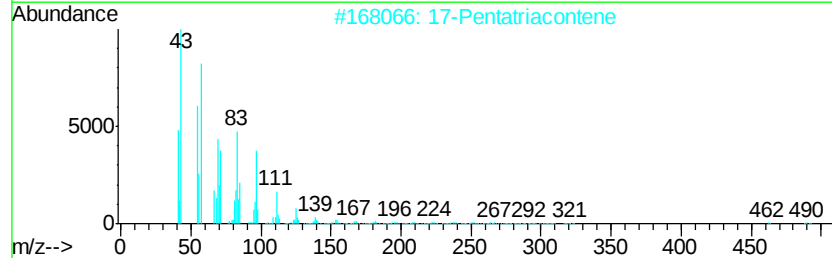
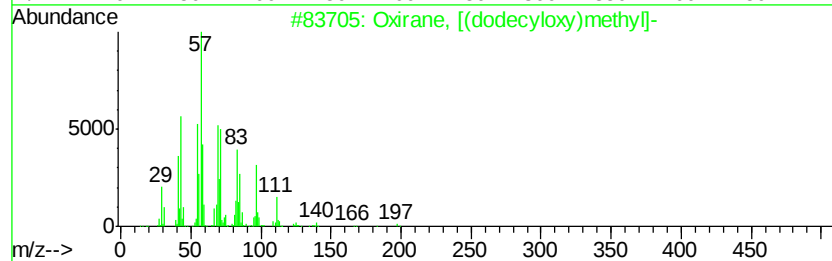
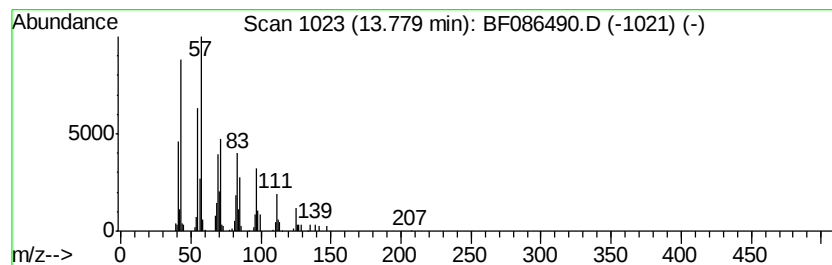
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Oxirane, [(dodecyloxy)methyl]- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.78	2.17 ng	147722	Chrysene-d12		13.93	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Oxirane, [(dodecyloxy)methyl]-	242	C15H30O2	002461-18-9	91
2		17-Pentatriacontene	491	C35H70	006971-40-0	87
3		Pentafluoropropionic acid, octadecyl ester	416	C21H37F5O2	1000280-07-7	72
4		Trichloroacetic acid, pentadecyl ester	372	C17H31Cl3O2	074339-53-0	72
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	4.27	47.5	ng	2520410	1	6.77	1062220	20.0
2-Pentanone, 4-hy...	4.94	68.6	ng	3642100	1	6.77	1062220	20.0
2-Pentanone, 4-me...	5.78	11.9	ng	630198	1	6.77	1062220	20.0
unknown6.54	6.54	47.4	ng	2516360	1	6.77	1062220	20.0
Oxirane, [(dodecy...	13.78	2.2	ng	147722	5	13.93	1363700	20.0