

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060416\
 Data File : BF087690.D
 Acq On : 5 Jun 2016 5:40
 Operator : UM/SJ
 Sample : H3344-02
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-13

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-BF060416.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	1.770	15	16	26	rVB	362003	614185	14.00%	1.782%
2	1.907	26	28	46	rVB	2295387	4386262	100.00%	12.724%
3	2.135	46	48	69	rVB	106347	361852	8.25%	1.050%
4	5.039	299	302	307	rVB	137127	170440	3.89%	0.494%
5	5.450	335	338	340	rBV	1857846	1790105	40.81%	5.193%
6	6.479	425	428	430	rBV	1351189	1265243	28.85%	3.670%
7	6.627	438	441	443	rBV	2621887	3242064	73.91%	9.405%
8	6.856	459	461	465	rVB	937246	810586	18.48%	2.351%
9	7.016	472	475	477	rBV	2930509	2801967	63.88%	8.128%
10	7.427	508	511	513	rVB	2183835	2676245	61.01%	7.764%
11	8.147	571	574	576	rBV	924841	1077617	24.57%	3.126%
12	8.673	618	620	623	rBV	49454	74382	1.70%	0.216%
13	9.222	665	668	671	rVB	3237202	4227553	96.38%	12.264%
14	9.610	700	702	704	rBV	52310	58733	1.34%	0.170%
15	9.896	725	727	729	rVB	1259623	1165466	26.57%	3.381%
16	10.079	740	743	746	rBV	37292	57288	1.31%	0.166%
17	10.685	793	796	799	rBV	2180247	2589113	59.03%	7.511%
18	10.811	805	807	811	rVB	29804	45125	1.03%	0.131%
19	11.256	842	846	851	rBV4	28705	59104	1.35%	0.171%
20	11.382	854	857	859	rVB	1262864	1238435	28.23%	3.593%
21	11.908	902	903	906	rBV	69402	98895	2.25%	0.287%
22	12.696	970	972	978	rBV	112905	149926	3.42%	0.435%
23	12.799	978	981	983	rVB	70293	70239	1.60%	0.204%
24	12.971	993	996	998	rBV	3336608	3552607	80.99%	10.306%
25	13.497	1040	1042	1044	rBV	37820	44443	1.01%	0.129%
26	14.011	1084	1087	1089	rBV	1199571	1078428	24.59%	3.128%
27	15.440	1209	1212	1215	rBV	634962	765165	17.44%	2.220%

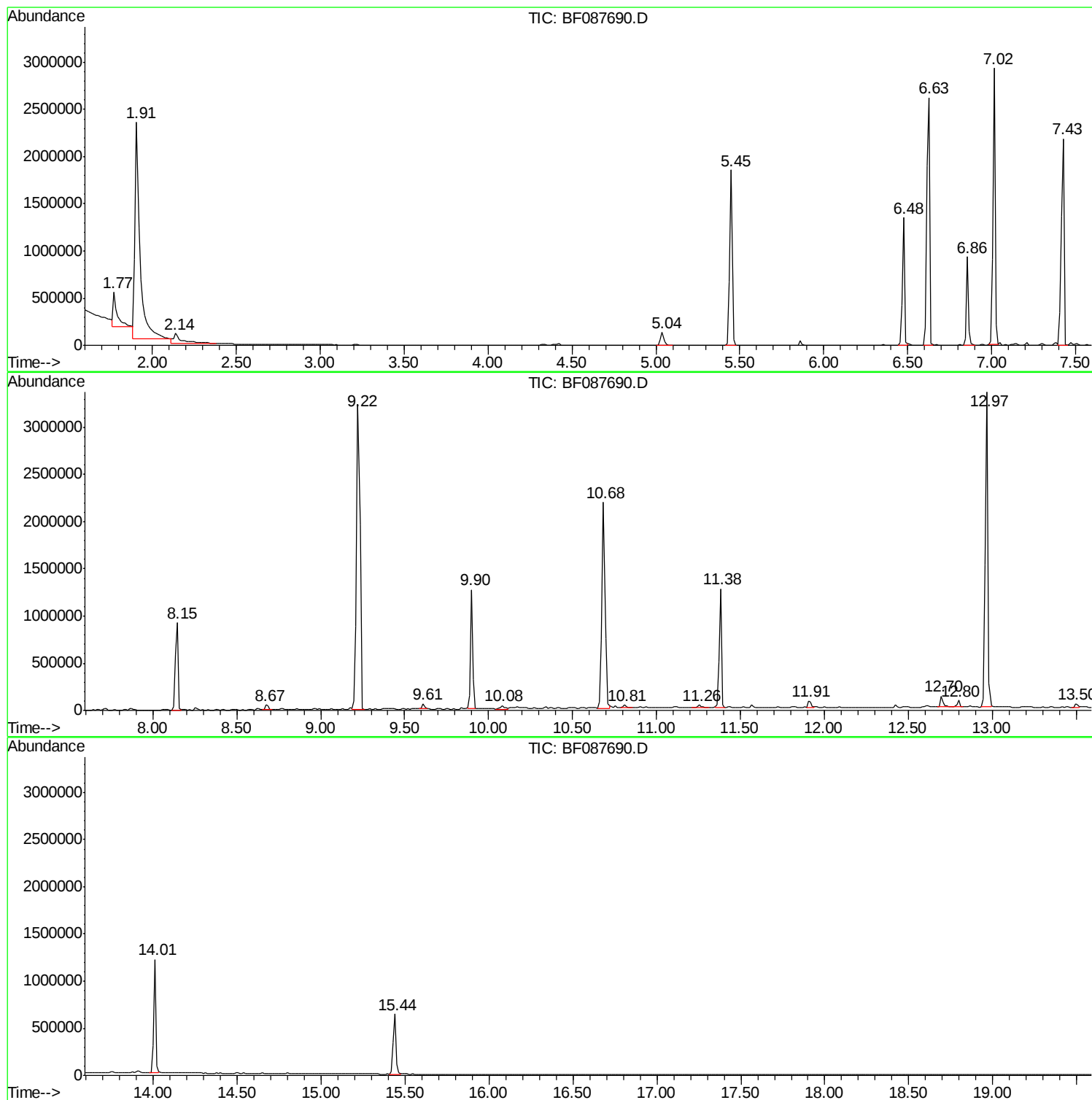
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



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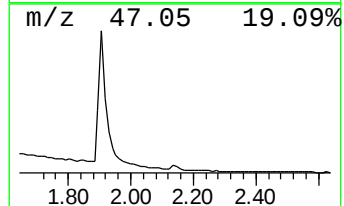
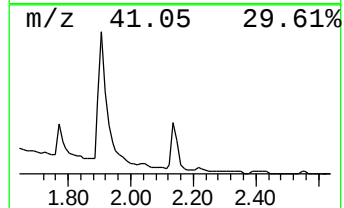
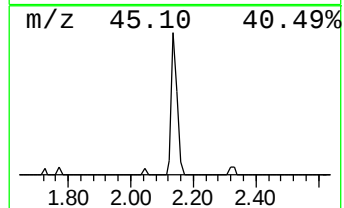
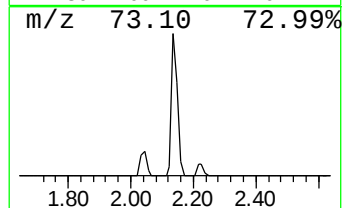
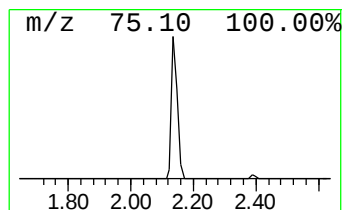
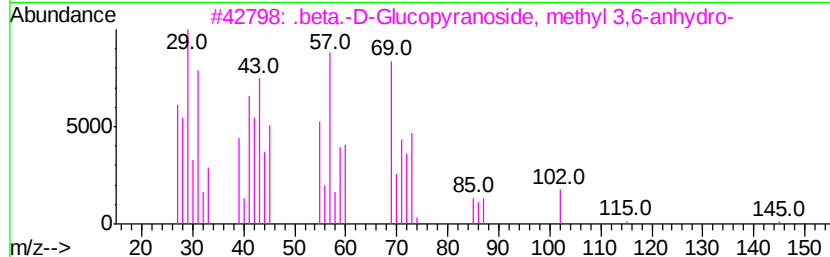
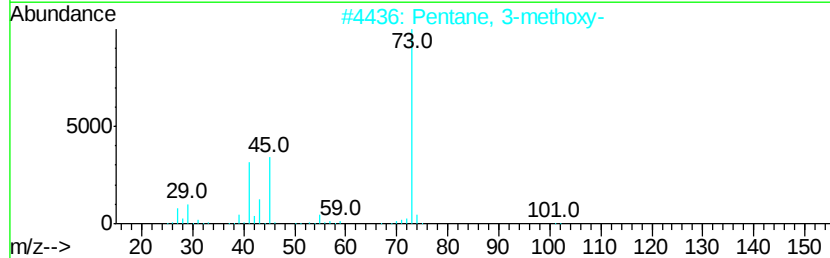
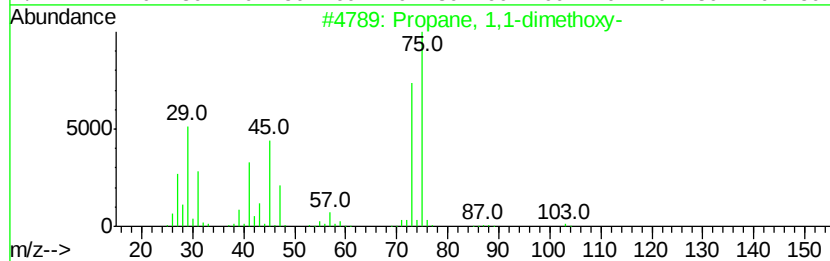
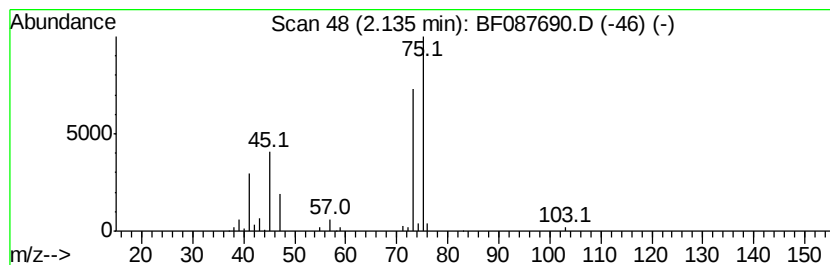
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	8.93 ng	361852	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3		.beta.-D-Glucopyranoside, methyl...	176	C7H12O5	003056-46-0	9
4		Propane, 1,1-dimethoxy-2-methyl-	118	C6H14O2	041632-89-7	9
5		Ethane, 2-chloro-1,1-dimethoxy-	124	C4H9ClO2	000097-97-2	9



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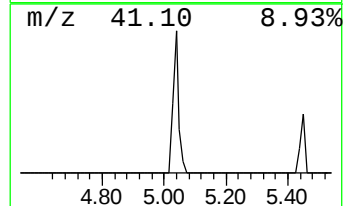
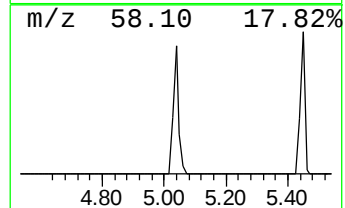
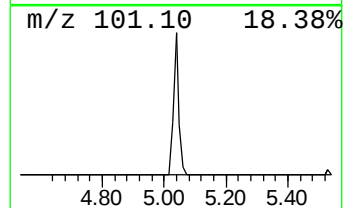
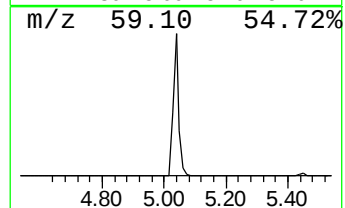
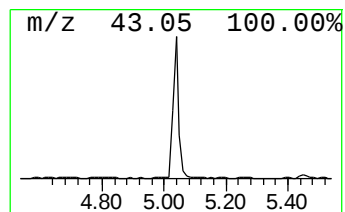
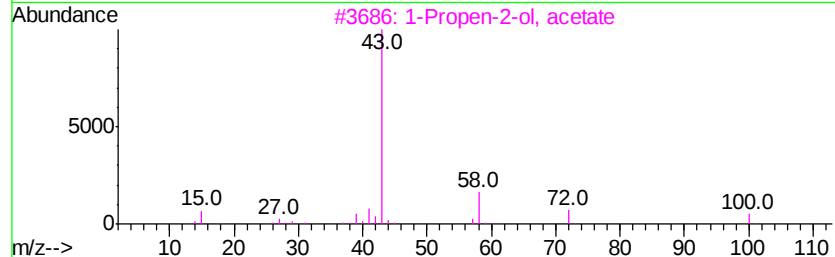
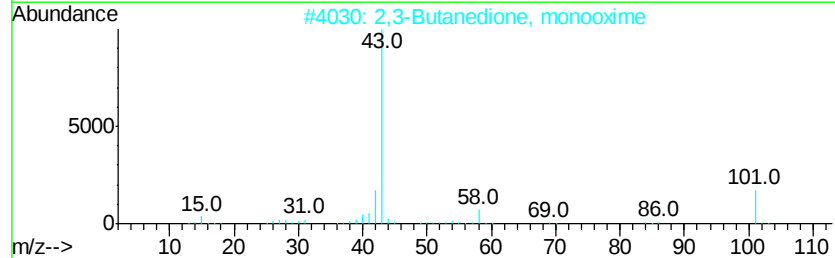
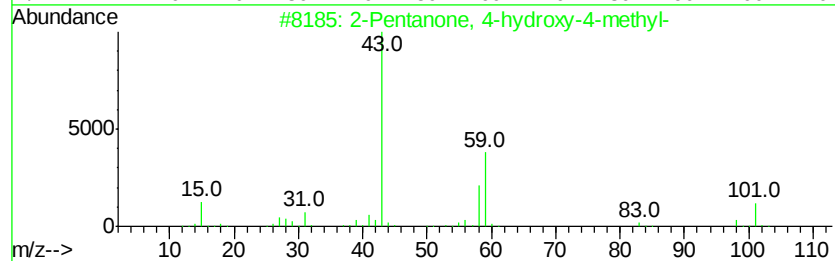
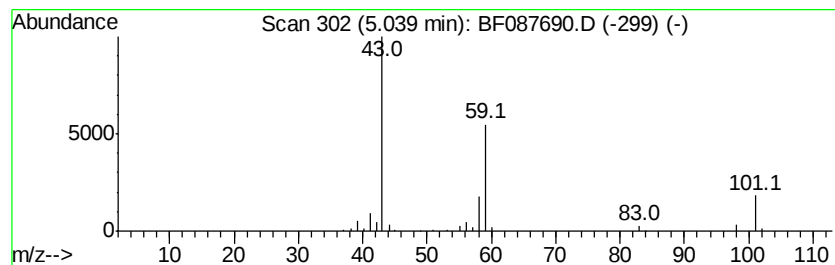
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	4.21 ng	170440	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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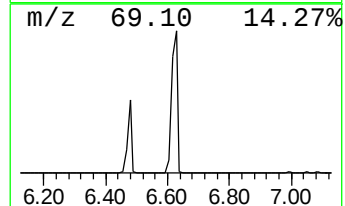
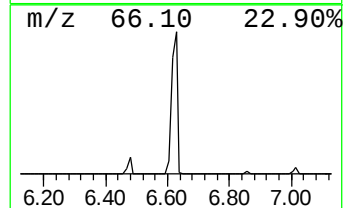
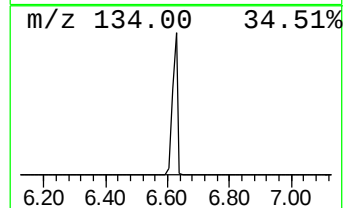
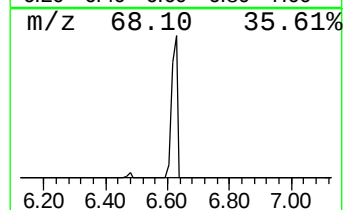
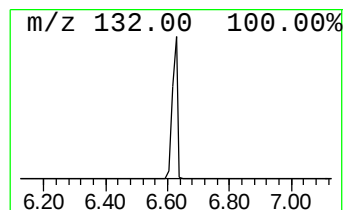
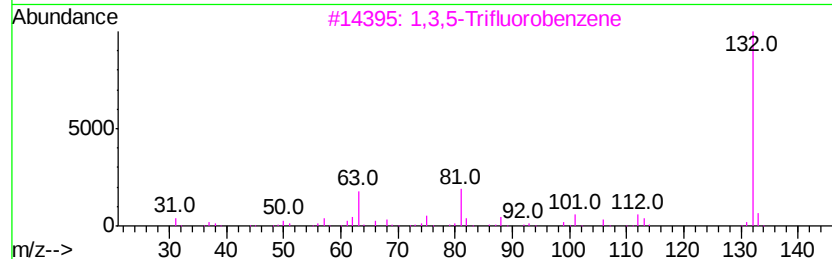
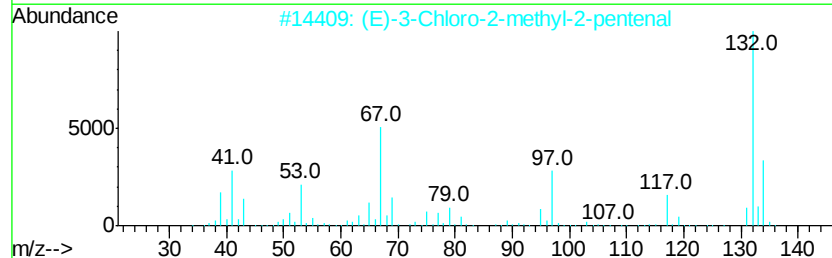
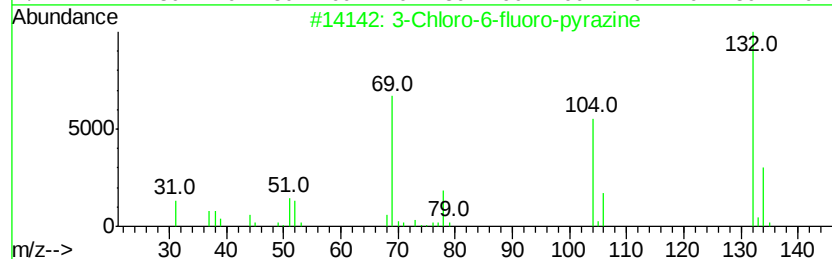
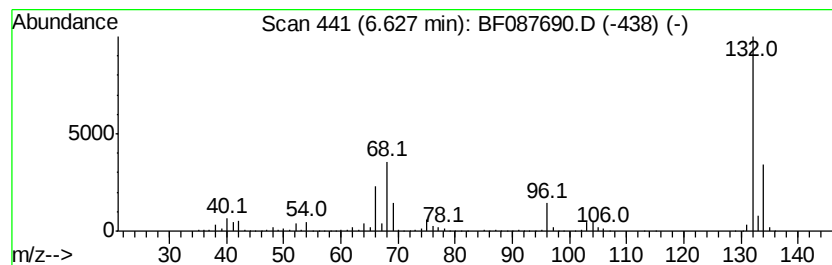
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Peak Number 5 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	79.99 ng	3242060	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine			132	C4H2ClFN2	1000146-10-7	35
2	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	17
3	1,3,5-Trifluorobenzene			132	C6H3F3	000372-38-3	9
4	5-Fluoro-2-chloropyrimidine			132	C4H2ClFN2	062802-42-0	9
5	1H-Benzimidazole, 2-methyl-			132	C8H8N2	000615-15-6	9



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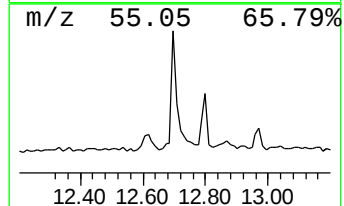
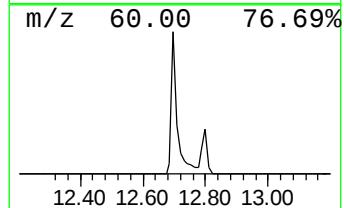
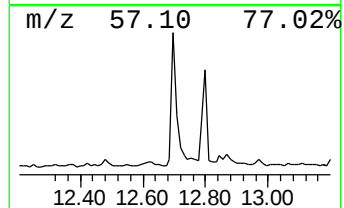
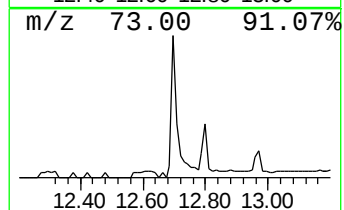
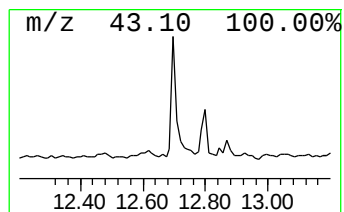
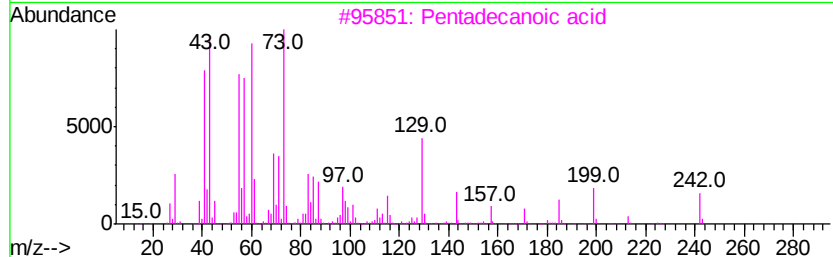
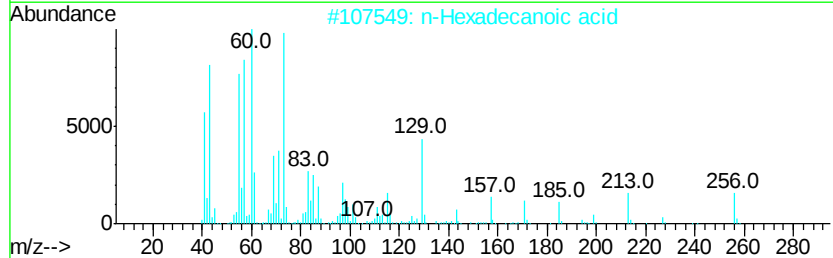
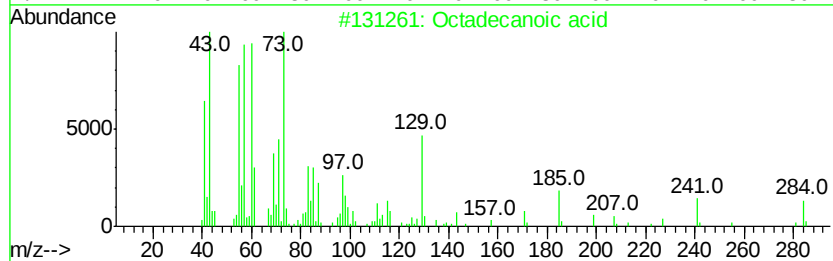
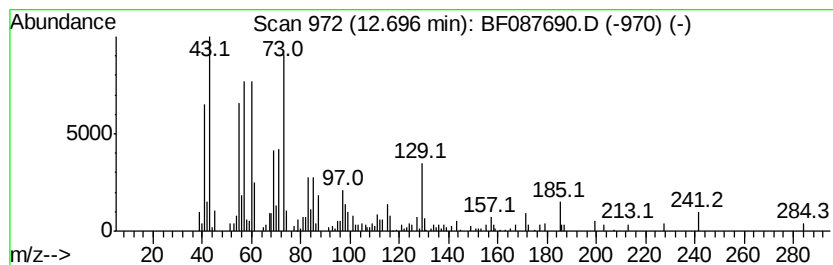
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Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.70	2.42 ng	149926	Phenanthrene-d10	11.38

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
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	60



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.14	8.9	ng	361852	1	6.86	810586	20.0
2-Pentanone, 4-hy...	5.04	4.2	ng	170440	1	6.86	810586	20.0
unknown6.63	6.63	80.0	ng	3242060	1	6.86	810586	20.0
Octadecanoic acid	12.70	2.4	ng	149926	4	11.38	1238440	20.0