

Data Path : Z:\HPCHEM1\BNA F\DATA\BF030917\
 Data File : BF093494.D
 Acq On : 9 Mar 2017 23:57
 Operator : SJ/MA
 Sample : I2211-06
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-2-TP-1-COMP-0-12FT

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-BF030717.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	1.956	3	6	18	rVB	84391	200007	4.09%	0.467%
2	4.904	262	264	280	rBV	650475	1071645	21.90%	2.501%
3	5.350	301	303	321	rBV	3598608	4892486	100.00%	11.420%
4	6.402	393	395	403	rBV	3896519	4551635	93.03%	10.624%
5	6.516	403	405	408	rVV	3505335	4279838	87.48%	9.990%
6	6.745	423	425	428	rBV	936000	1124508	22.98%	2.625%
7	6.905	436	439	441	rBV	3678590	3347997	68.43%	7.815%
8	7.327	473	476	478	rBV	2350762	3090882	63.18%	7.215%
9	8.036	535	538	549	rBV	1617227	1520672	31.08%	3.550%
10	9.111	629	632	634	rBV	4528314	4593293	93.88%	10.722%
11	9.511	664	667	669	rBV	465775	423741	8.66%	0.989%
12	9.785	689	691	693	rBV	1704618	1608970	32.89%	3.756%
13	10.208	727	728	730	rVB	92778	99138	2.03%	0.231%
14	10.425	744	747	751	rBV	37293	70409	1.44%	0.164%
15	10.574	758	760	763	rBV	2268605	2459882	50.28%	5.742%
16	10.688	768	770	777	rVB	147327	208268	4.26%	0.486%
17	11.134	807	809	810	rBV	106944	102683	2.10%	0.240%
18	11.271	819	821	823	rBV	1668876	1652566	33.78%	3.857%
19	12.848	957	959	962	rBV	3427234	4240480	86.67%	9.898%
20	13.762	1036	1039	1046	rBV	100441	254037	5.19%	0.593%
21	13.911	1050	1052	1054	rBV	1526206	1594553	32.59%	3.722%
22	15.317	1172	1175	1187	rVB	979916	1318812	26.96%	3.078%
23	15.694	1205	1208	1211	rBV	43334	62401	1.28%	0.146%
24	16.140	1244	1247	1254	rVB	34752	72830	1.49%	0.170%

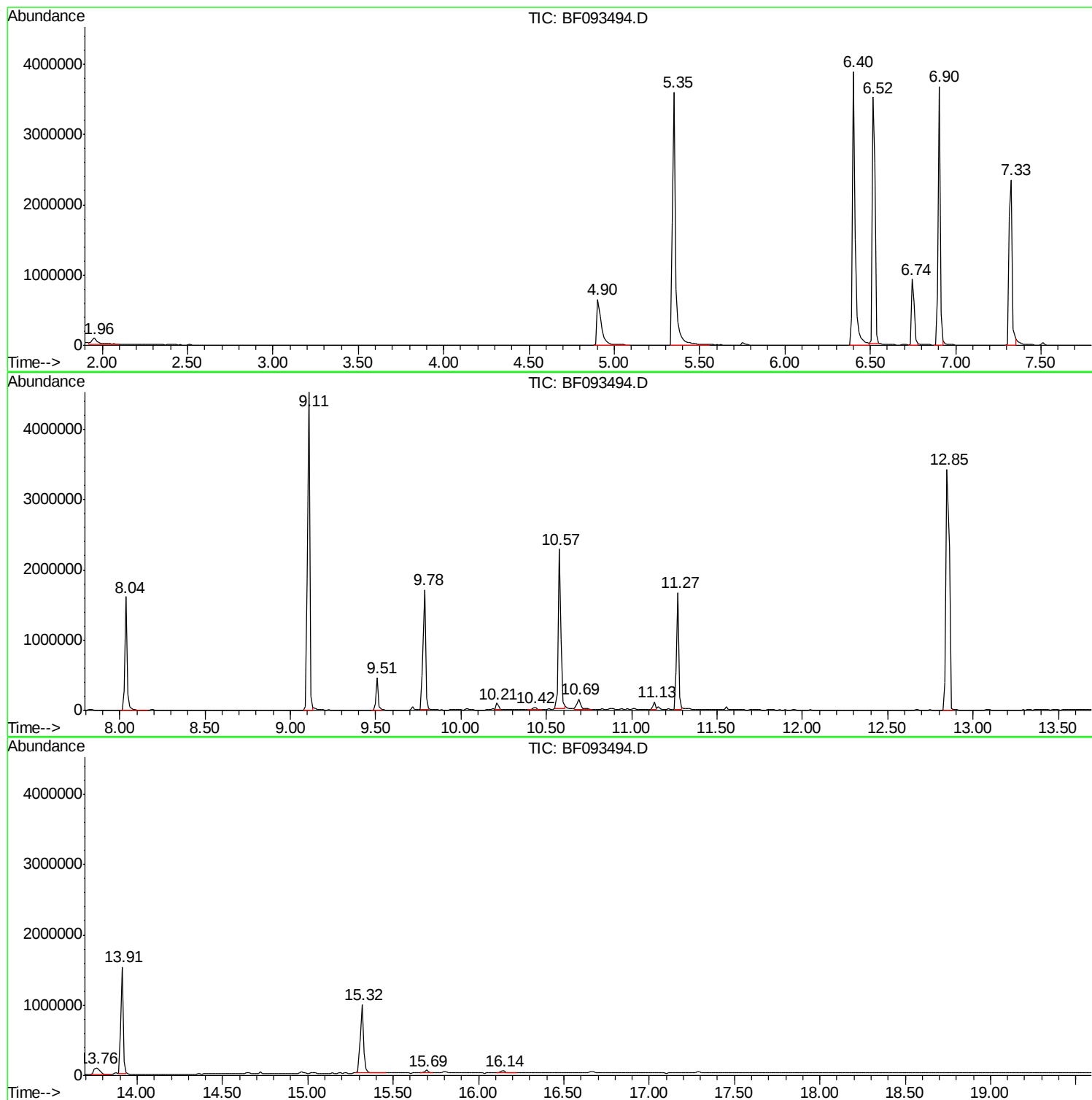
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF030717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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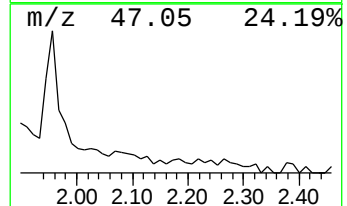
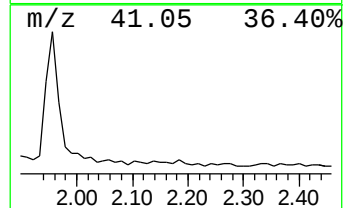
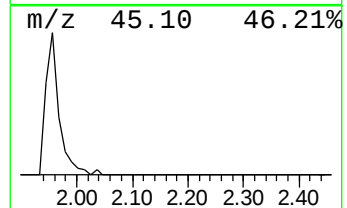
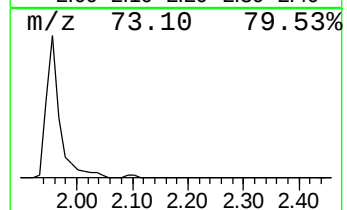
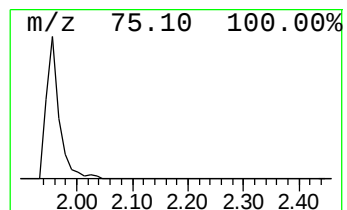
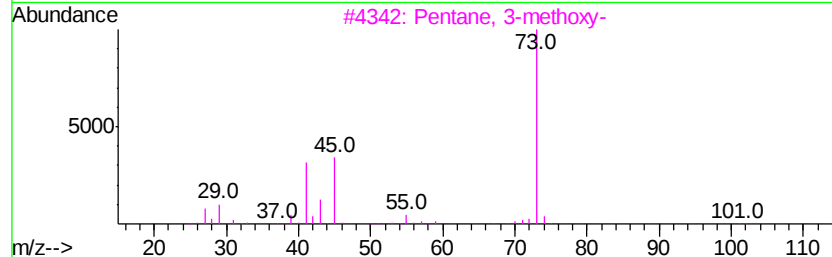
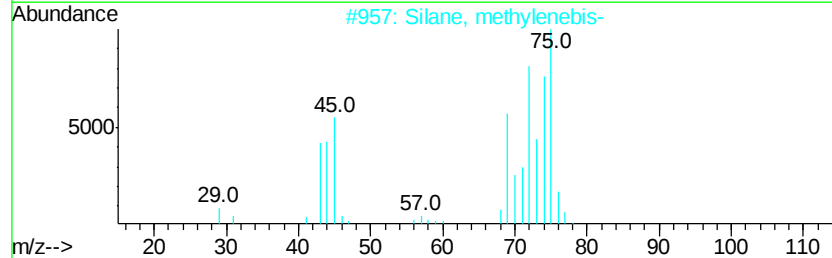
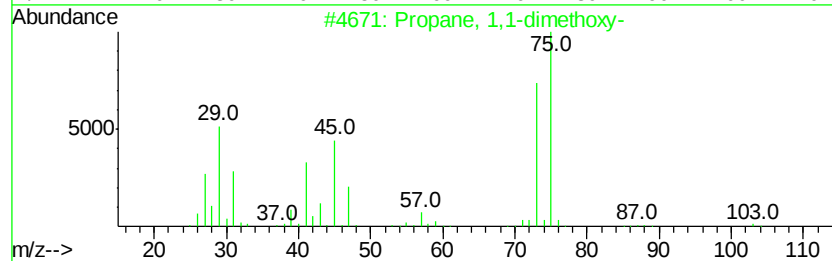
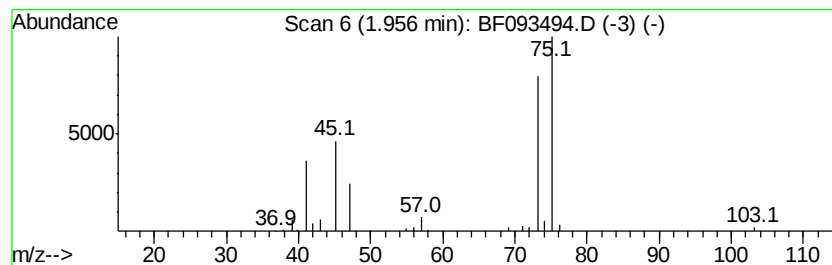
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.96	3.56 ng	200007	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	78
2		Silane, methylenebis-	76	CH8Si2	001759-88-2	50
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
4		Glycine	75	C2H5NO2	000056-40-6	9
5		2,2'-Bi-1,3-dioxolane	146	C6H10O4	006705-89-1	9



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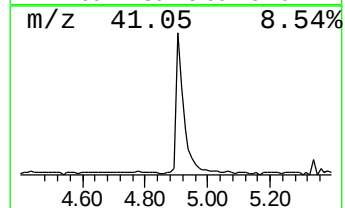
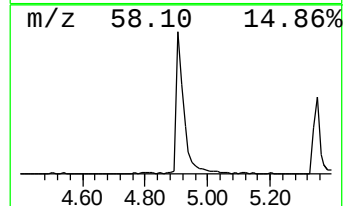
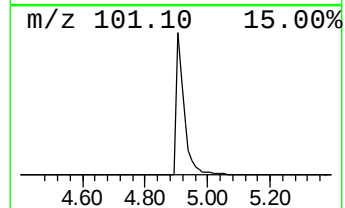
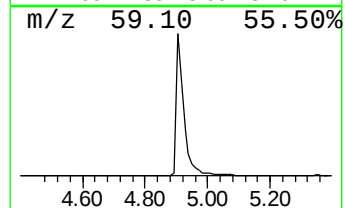
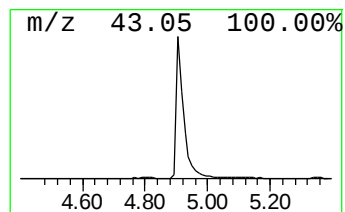
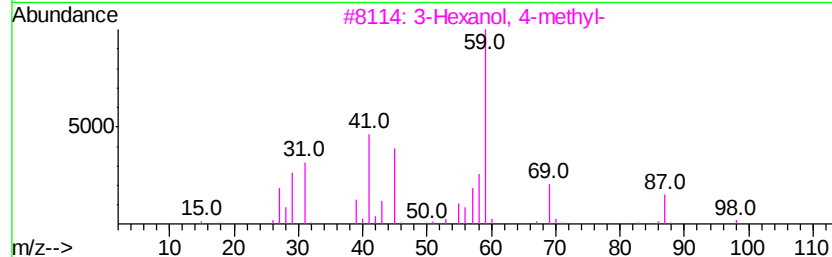
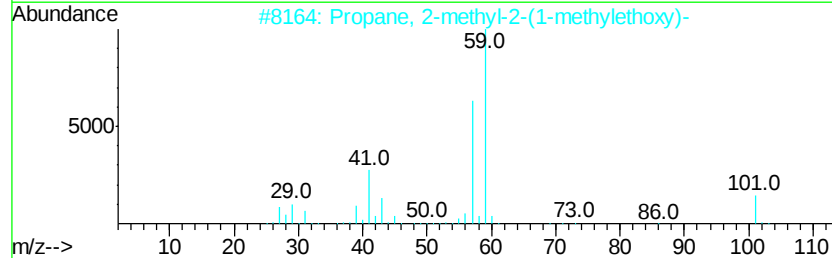
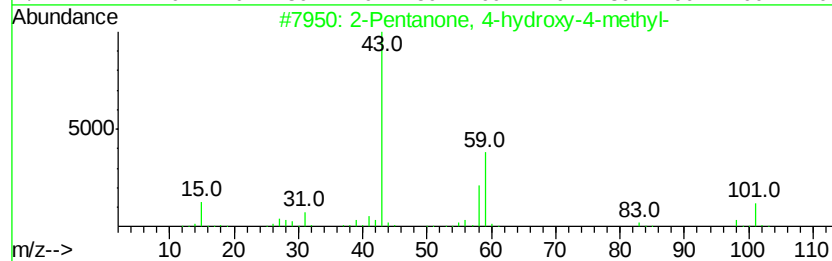
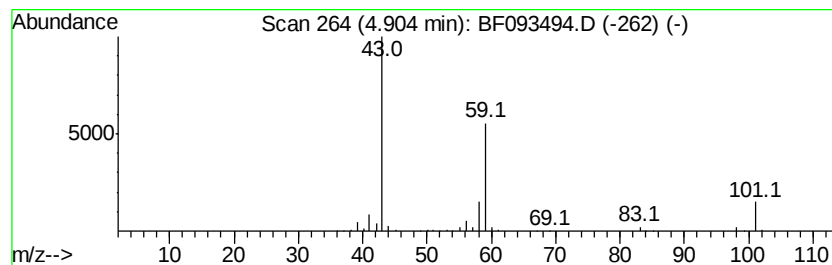
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.90	19.06 ng	1071650	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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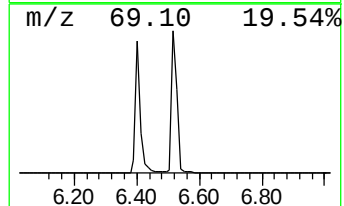
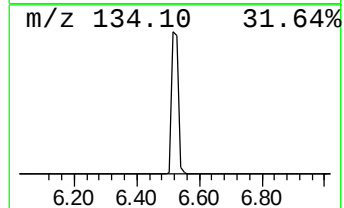
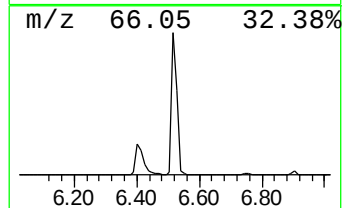
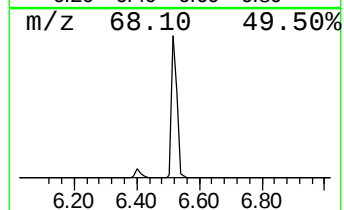
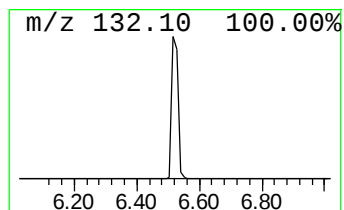
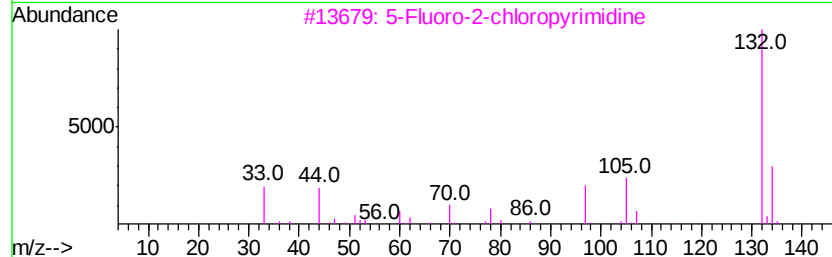
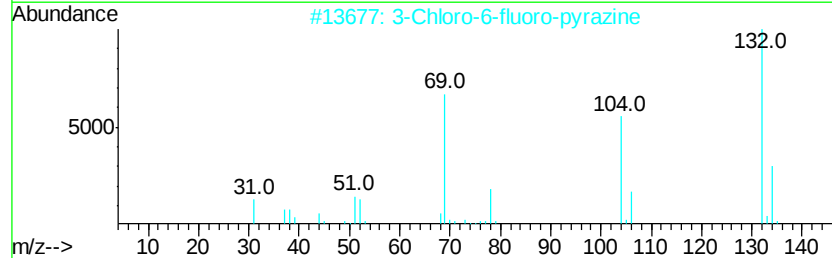
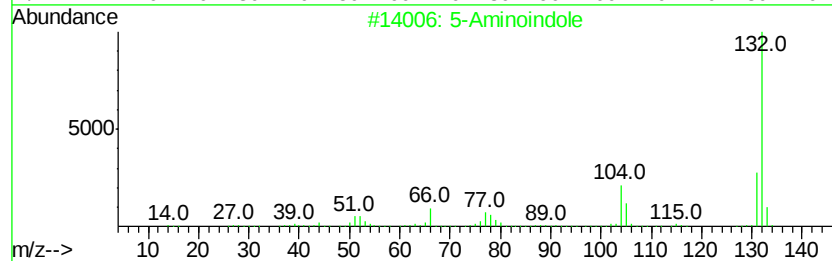
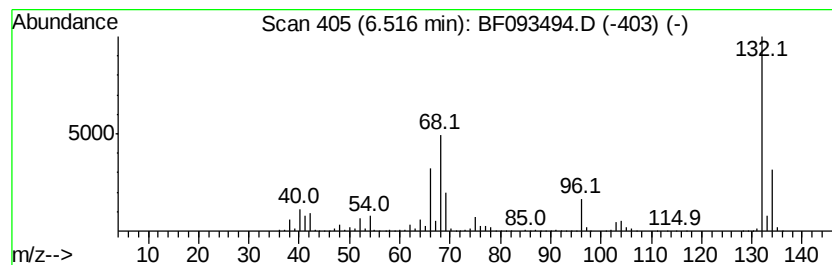
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Peak Number 3 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	76.12 ng	4279840	1,4-Dichlorobenzene-d4	6.74

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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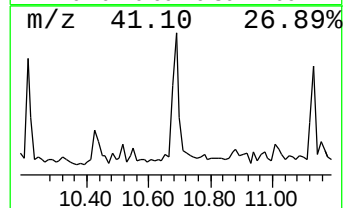
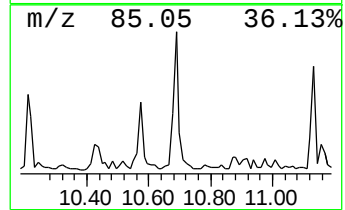
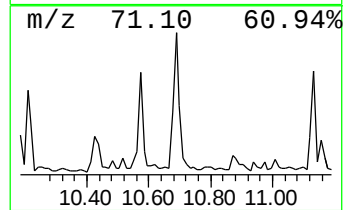
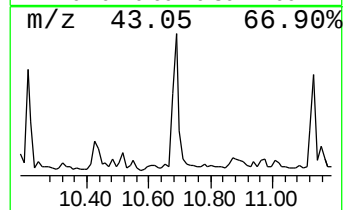
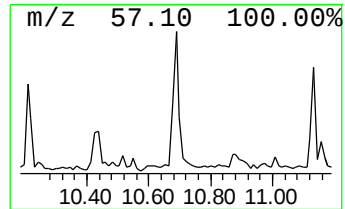
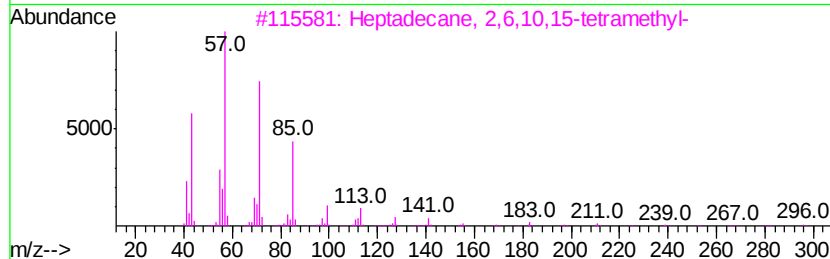
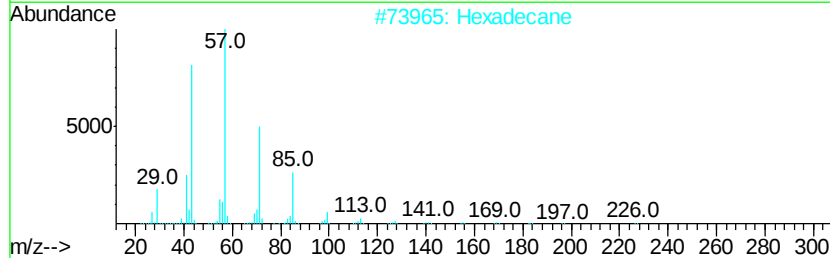
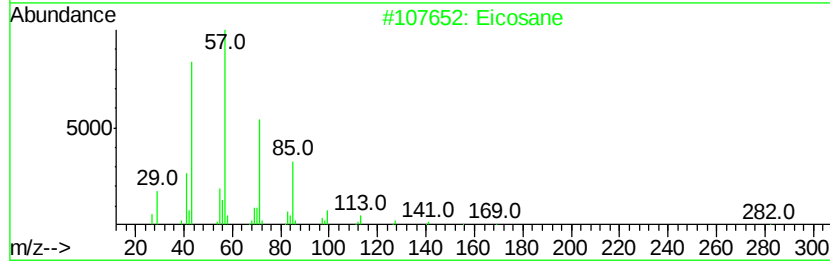
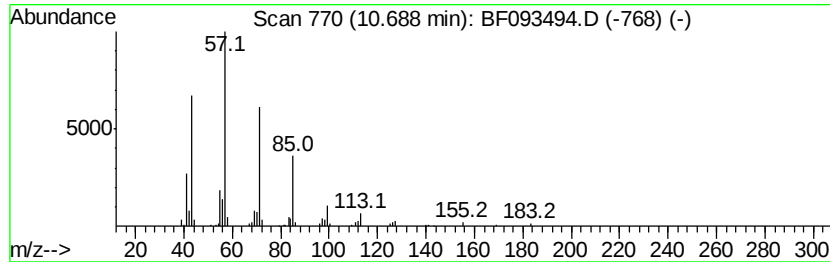
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Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.69	2.52 ng	208268	Phenanthrene-d10	11.27	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	91
2	Hexadecane	226	C16H34	000544-76-3	90
3	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Octadecane	254	C18H38	000593-45-3	86



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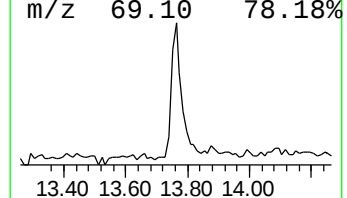
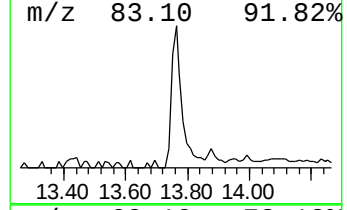
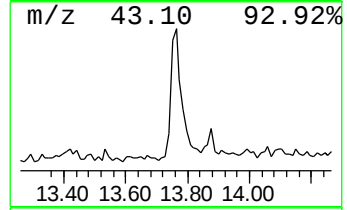
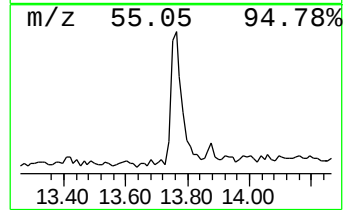
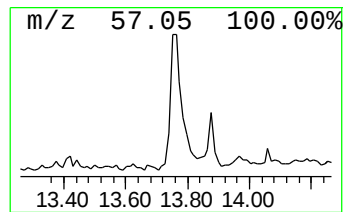
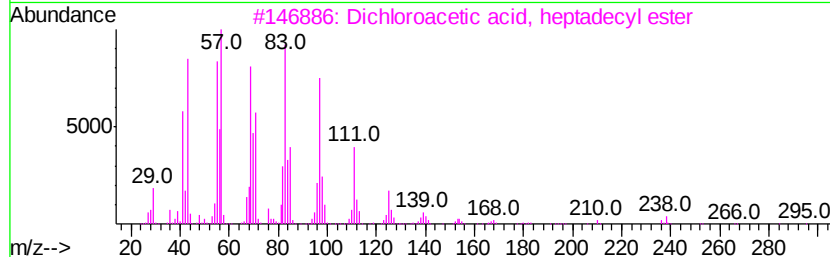
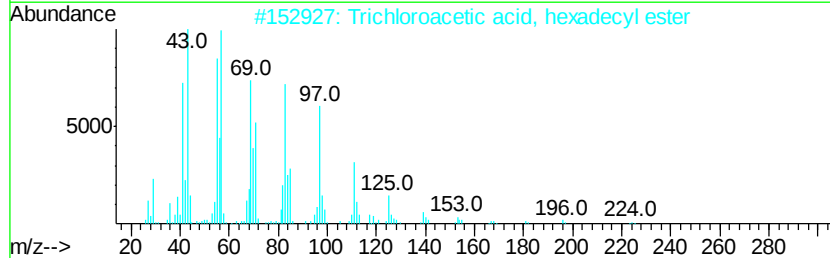
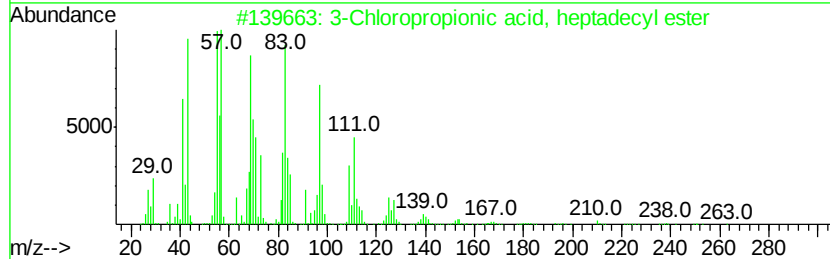
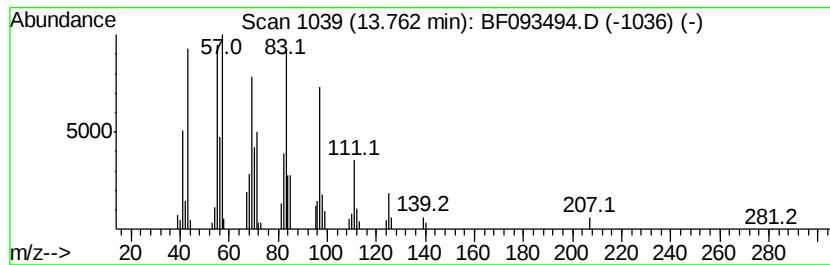
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 3-Chloropropionic acid, hep... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.76	3.19 ng	254037	Chrysene-d12	13.91

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	94
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
4		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	1.96	3.6	ng	200007	1	6.74	1124510	20.0
2-Pentanone, 4-hy...	4.90	19.1	ng	1071650	1	6.74	1124510	20.0
unknown6.52	6.52	76.1	ng	4279840	1	6.74	1124510	20.0
Eicosane	10.69	2.5	ng	208268	4	11.27	1652570	20.0
3-Chloropropionic...	13.76	3.2	ng	254037	5	13.91	1594550	20.0