

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF061116\
 Data File : BF087918.D
 Acq On : 11 Jun 2016 23:00
 Operator : UM/SJ
 Sample : H3362-05
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP16-MMW0002

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.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	1.735	12	13	22	rVB	398461	612378	13.66%	1.631%
2	1.861	22	24	37	rVV	2478294	4277966	95.40%	11.392%
3	2.021	37	38	79	rVB3	136019	843429	18.81%	2.246%
4	4.959	293	295	301	rVB	94427	124738	2.78%	0.332%
5	5.393	330	333	335	rBV	1331872	1639943	36.57%	4.367%
6	6.433	421	424	426	rBV	874337	1019215	22.73%	2.714%
7	6.570	433	436	438	rBV	2551961	2909250	64.88%	7.747%
8	6.799	454	456	458	rBV	1132256	938347	20.93%	2.499%
9	6.959	467	470	472	rVB	2744994	2620287	58.44%	6.978%
10	7.370	503	506	508	rBV	2039471	2334353	52.06%	6.216%
11	8.090	566	569	571	rBV	1410941	1345657	30.01%	3.584%
12	9.176	660	664	666	rBV	3102753	4484030	100.00%	11.941%
13	9.839	720	722	725	rVB2	1372264	1516320	33.82%	4.038%
14	10.628	788	791	794	rBV2	1747039	2630460	58.66%	7.005%
15	11.325	849	852	854	rBV	1850930	1646058	36.71%	4.383%
16	12.742	974	976	978	rBV	654203	533469	11.90%	1.421%
17	12.822	978	983	985	rVB2	40036	65242	1.45%	0.174%
18	12.914	988	991	994	rBV	2939254	4284800	95.56%	11.411%
19	13.451	1035	1038	1040	rBV	305379	372810	8.31%	0.993%
20	13.497	1040	1042	1045	rVB	29732	64465	1.44%	0.172%
21	13.954	1080	1082	1085	rBV	1402883	1553019	34.63%	4.136%
22	14.137	1096	1098	1100	rBV	63712	55611	1.24%	0.148%
23	14.742	1148	1151	1153	rBV	45944	57070	1.27%	0.152%
24	15.062	1176	1179	1181	rBV	45965	58046	1.29%	0.155%
25	15.371	1203	1206	1209	rBV	967126	1256809	28.03%	3.347%
26	15.417	1209	1210	1214	rVV	59055	64101	1.43%	0.171%
27	15.565	1215	1223	1229	rVV4	15643	83186	1.86%	0.222%
28	15.828	1243	1246	1249	rBV	35361	51487	1.15%	0.137%
29	16.297	1280	1287	1295	rBV2	27328	63526	1.42%	0.169%
30	17.497	1388	1392	1396	rBV4	12325	45295	1.01%	0.121%

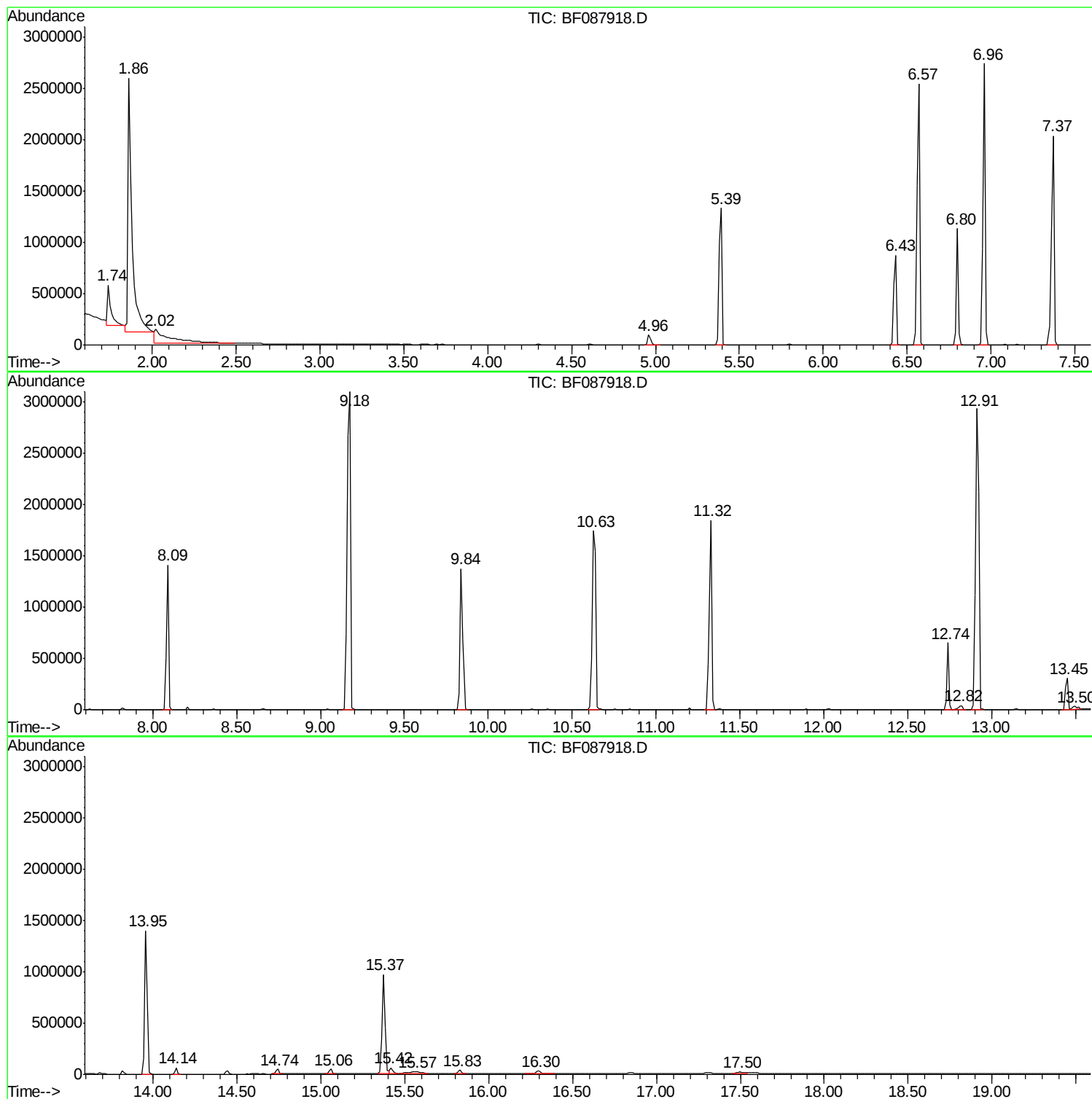
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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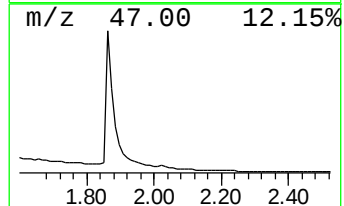
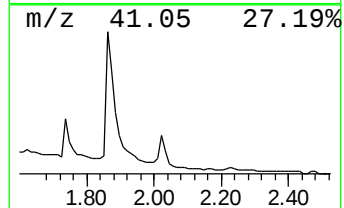
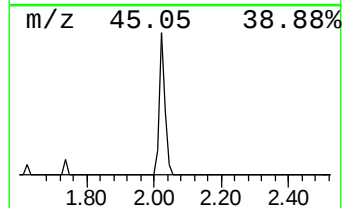
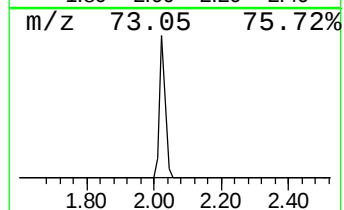
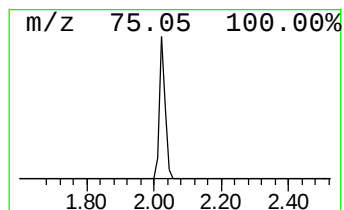
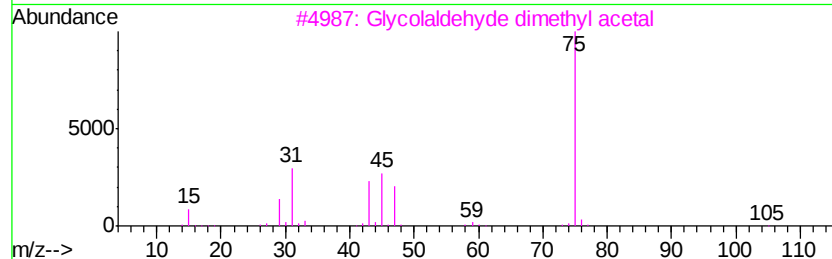
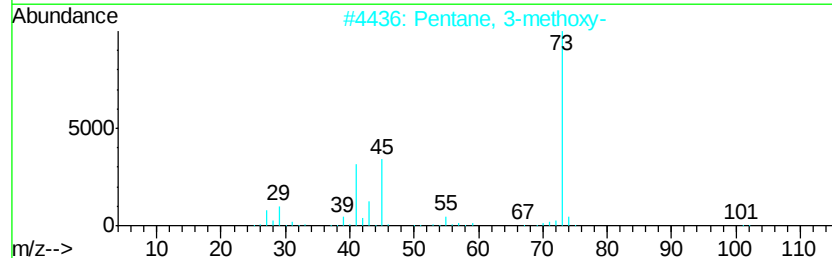
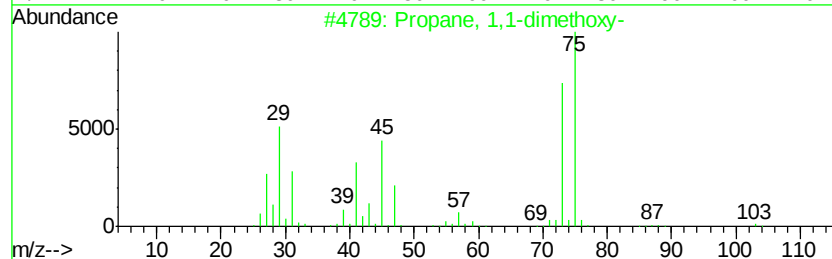
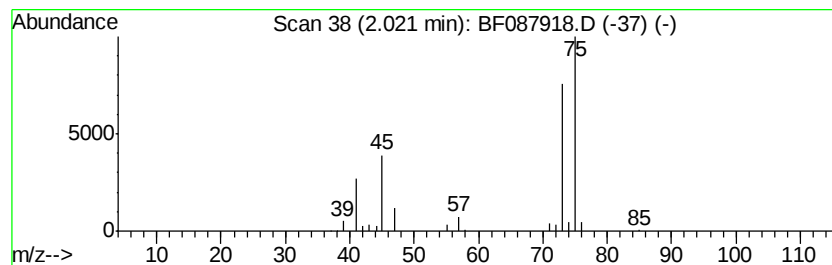
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Propane, 1,1-dimethoxy- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.02	17.98 ng	843429	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	72
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	27
3		Glycolaldehyde dimethyl acetal	106	C4H10O3	030934-97-5	9
4		1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5		1,3-Dioxolane, 2-(chloromethyl)-	122	C4H7ClO2	002568-30-1	9



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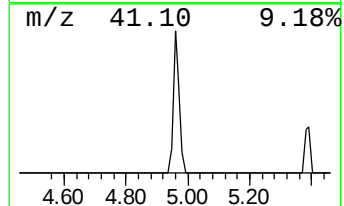
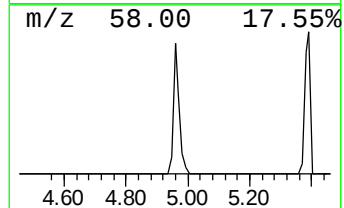
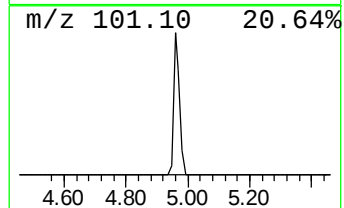
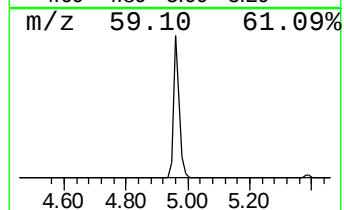
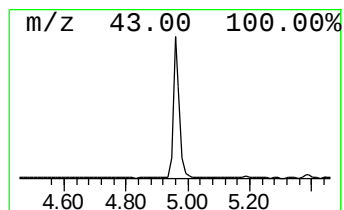
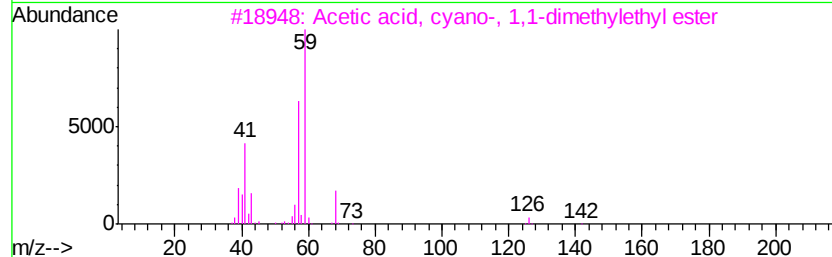
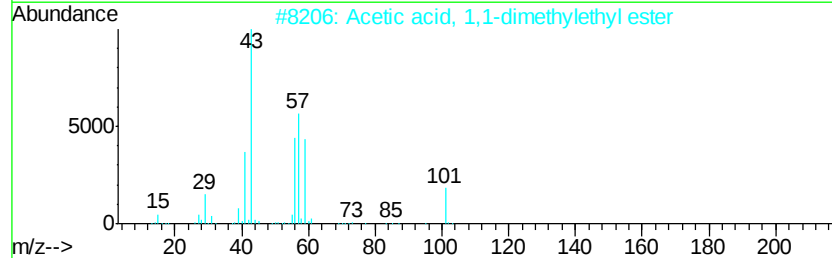
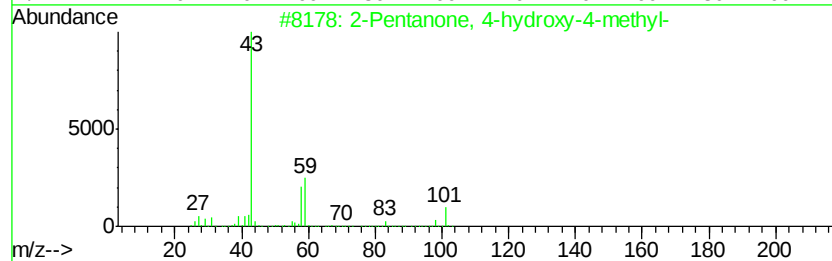
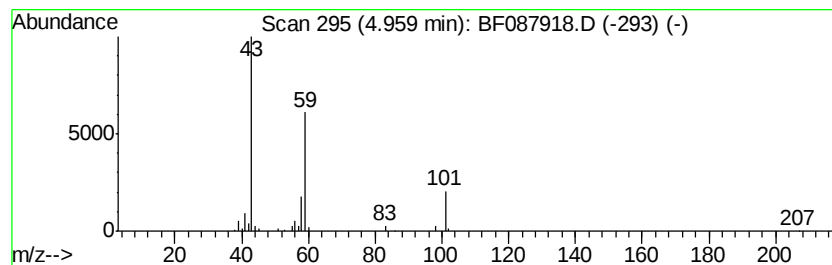
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	2.66 ng	124738	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		Acetone	58	C3H6O	000067-64-1	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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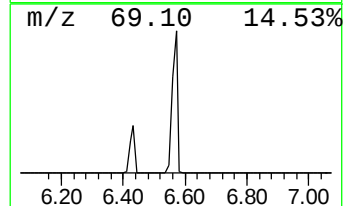
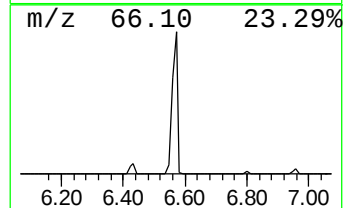
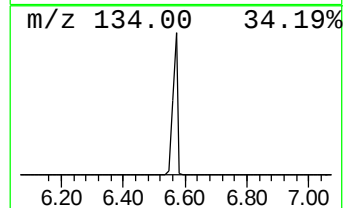
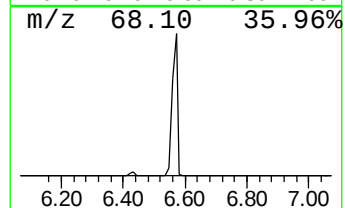
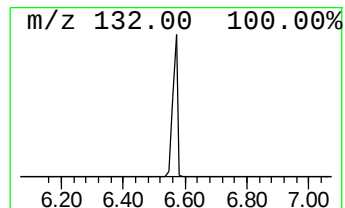
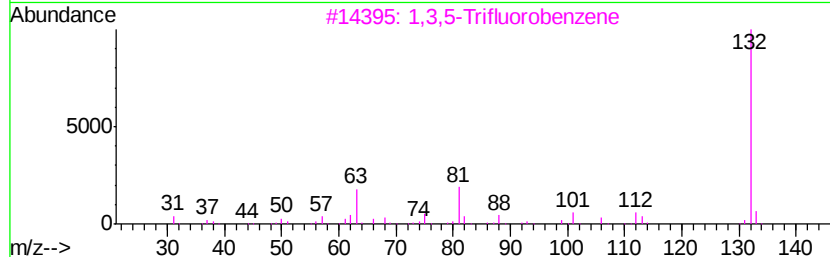
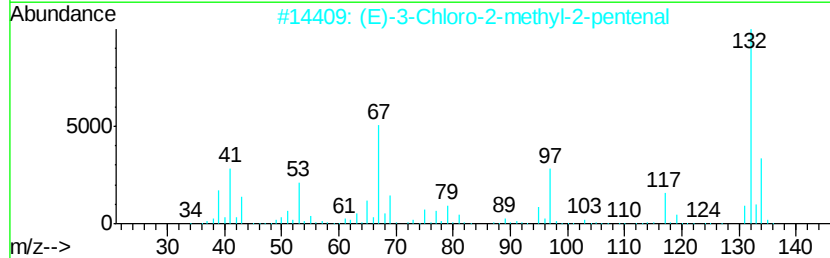
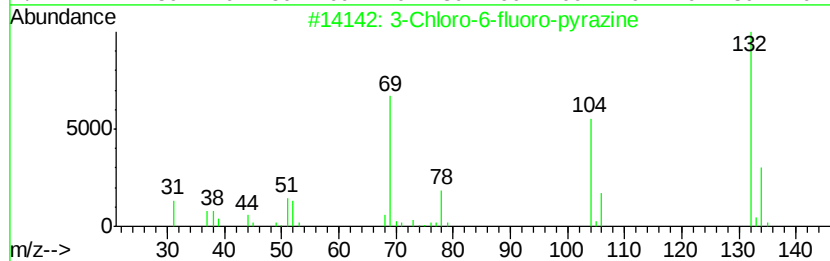
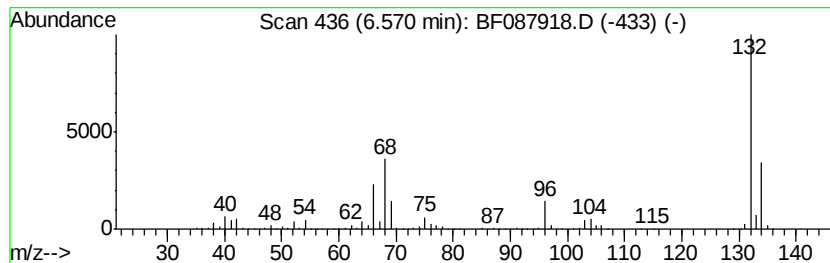
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Peak Number 5 unknown6.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	62.01 ng	2909250	1,4-Dichlorobenzene-d4	6.80

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	17
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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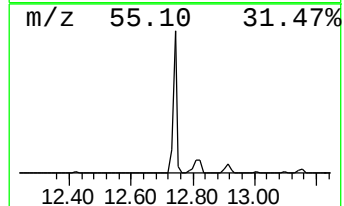
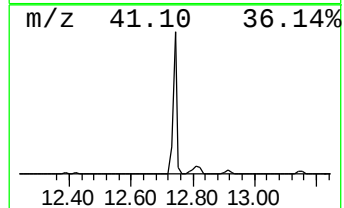
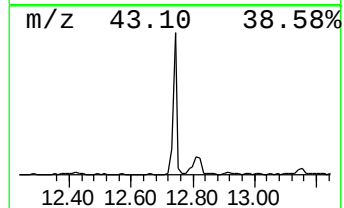
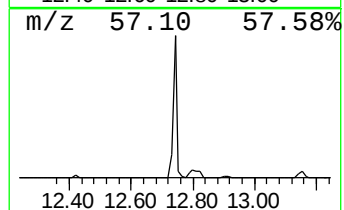
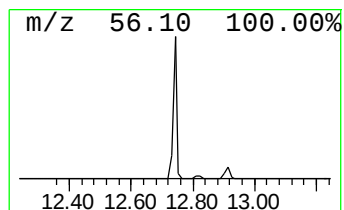
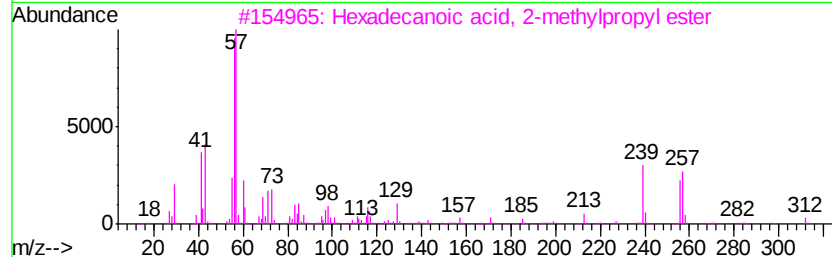
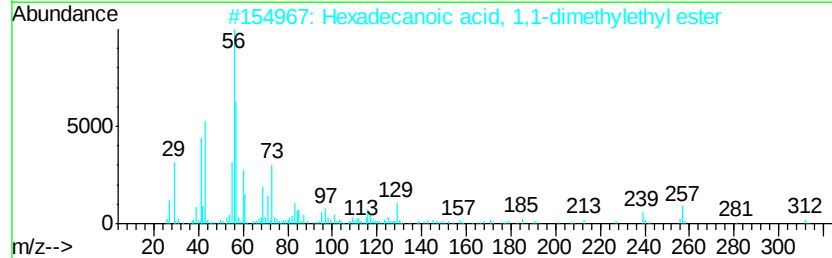
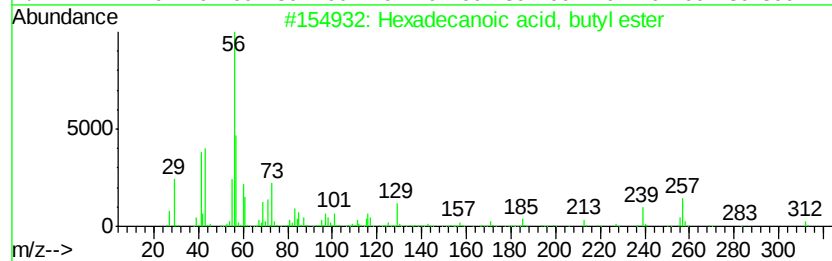
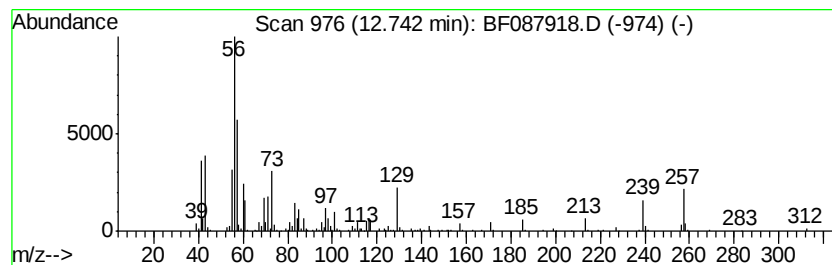
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Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.74	6.87 ng	533469	Chrysene-d12	13.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	72
3			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
4			Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35
5			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



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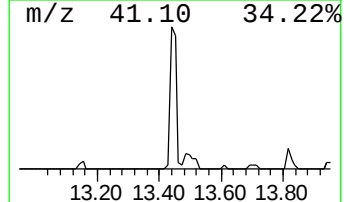
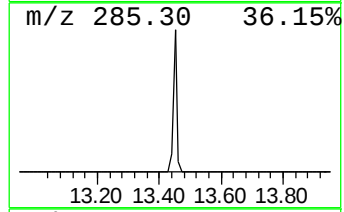
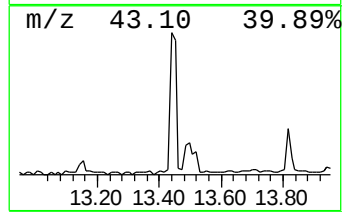
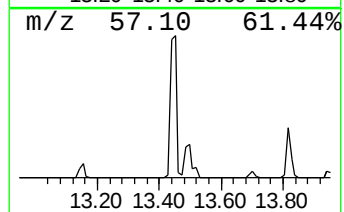
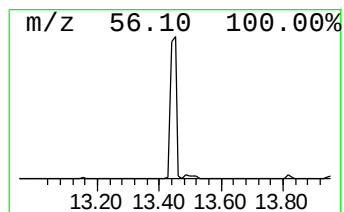
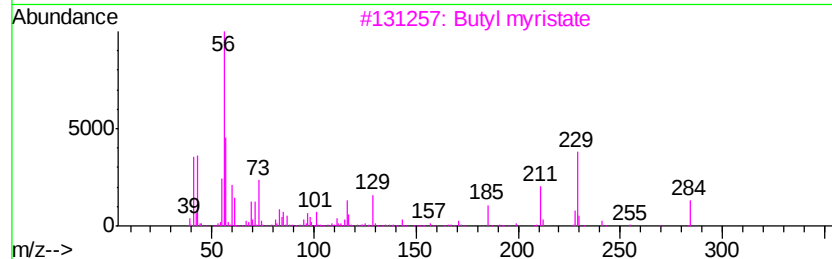
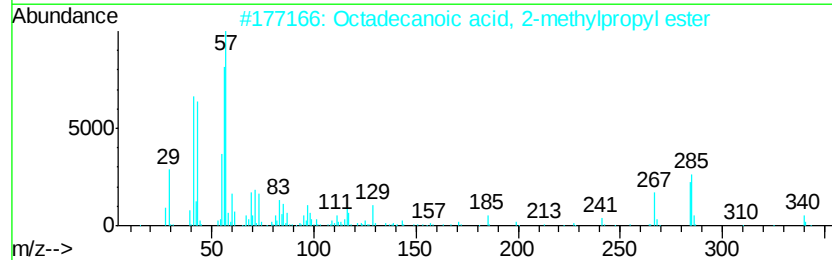
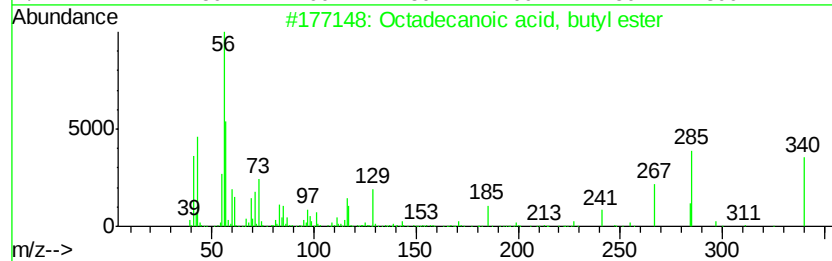
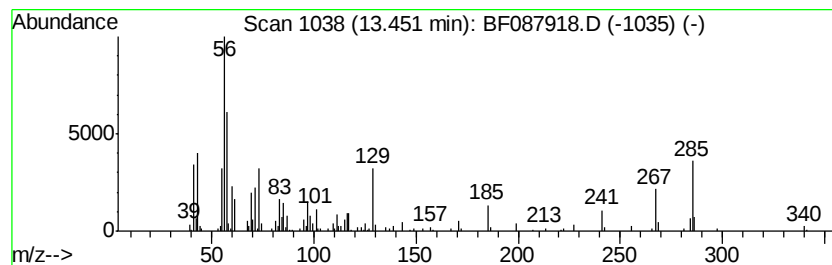
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TIC Library : C:\Database\NIST11.L
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Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.45	4.80 ng	372810	Chrysene-d12	13.95

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Octadecanoic acid, 2-methylpropyl...	340	C22H44O2	000646-13-9	87
3		Butyl myristate	284	C18H36O2	000110-36-1	47
4		Nipecotic acid	129	C6H11NO2	000498-95-3	43
5		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.02	18.0	ng	843429	1	6.80	938347	20.0
2-Pentanone, 4-hy...	4.96	2.7	ng	124738	1	6.80	938347	20.0
unknown6.57	6.57	62.0	ng	2909250	1	6.80	938347	20.0
Hexadecanoic acid...	12.74	6.9	ng	533469	5	13.95	1553020	20.0
Octadecanoic acid...	13.45	4.8	ng	372810	5	13.95	1553020	20.0