

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060516\
 Data File : BF087713.D
 Acq On : 5 Jun 2016 17:50
 Operator : UM/SJ
 Sample : H3362-05
 Misc :
 ALS Vial : 52 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-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	305688	522054	13.16%	1.636%
2	1.907	26	28	47	rVB	2014502	3639516	91.77%	11.404%
3	2.135	47	48	66	rVB2	65728	198520	5.01%	0.622%
4	5.039	300	302	306	rBV	99896	125100	3.15%	0.392%
5	5.450	335	338	341	rBV	1458997	1417654	35.74%	4.442%
6	6.479	426	428	431	rBV	1024223	890042	22.44%	2.789%
7	6.627	438	441	443	rBV	2785861	2927431	73.81%	9.172%
8	6.856	459	461	464	rBV	987591	891657	22.48%	2.794%
9	7.016	472	475	477	rBV	2777980	2589901	65.30%	8.115%
10	7.427	507	511	513	rBV	2064638	2434621	61.39%	7.628%
11	8.147	571	574	576	rBV	1185166	1269066	32.00%	3.976%
12	9.222	665	668	671	rBV	3098480	3966045	100.00%	12.427%
13	9.896	725	727	730	rVB	1371536	1348174	33.99%	4.224%
14	10.685	793	796	799	rBV	2053858	2339794	59.00%	7.331%
15	11.382	854	857	859	rBV	1634733	1443925	36.41%	4.524%
16	12.799	979	981	983	rBV	264074	233678	5.89%	0.732%
17	12.971	993	996	999	rBV	3208591	3493188	88.08%	10.945%
18	13.497	1040	1042	1045	rBV	134819	150569	3.80%	0.472%
19	14.011	1084	1087	1090	rBV	1241963	1140249	28.75%	3.573%
20	15.440	1209	1212	1215	rBV	730215	894353	22.55%	2.802%

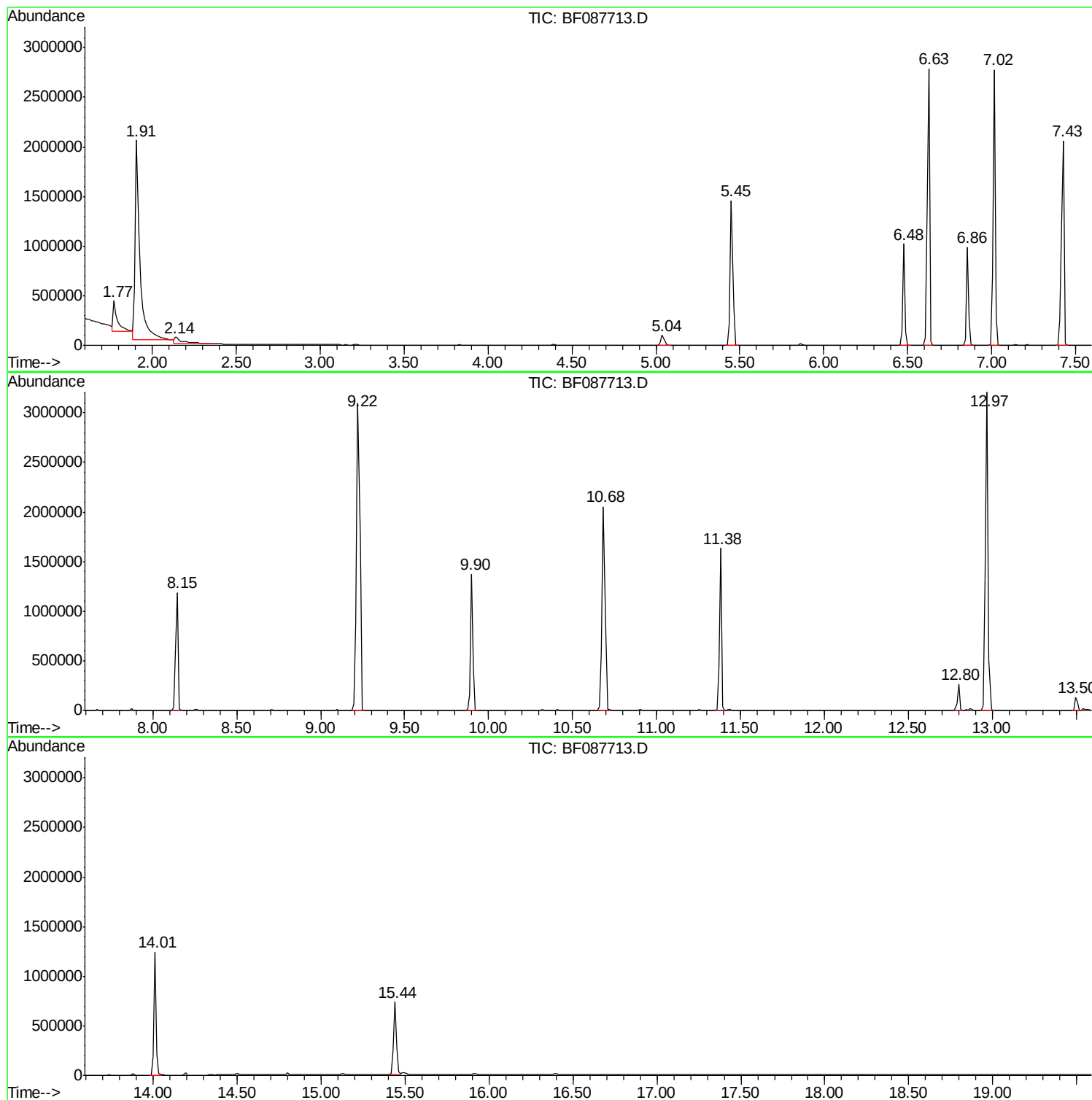
Sum of corrected areas: 31915537

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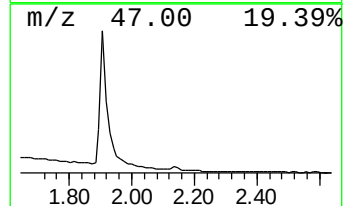
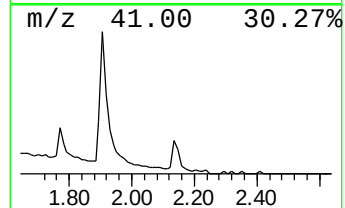
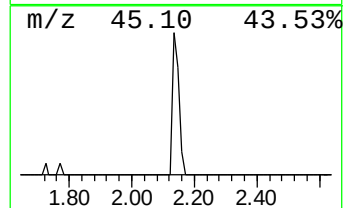
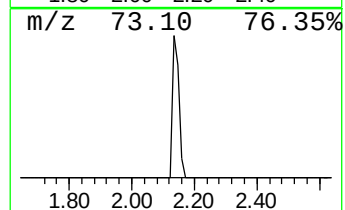
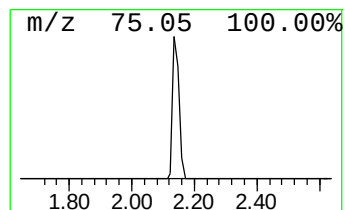
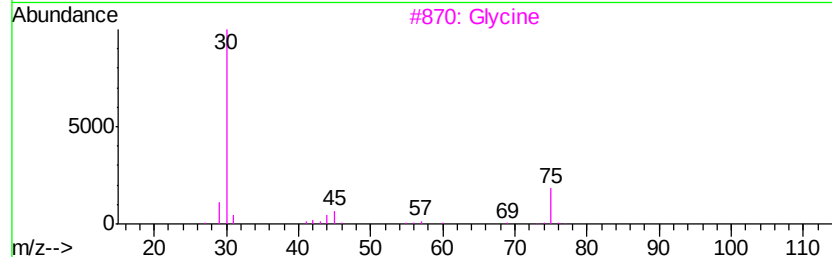
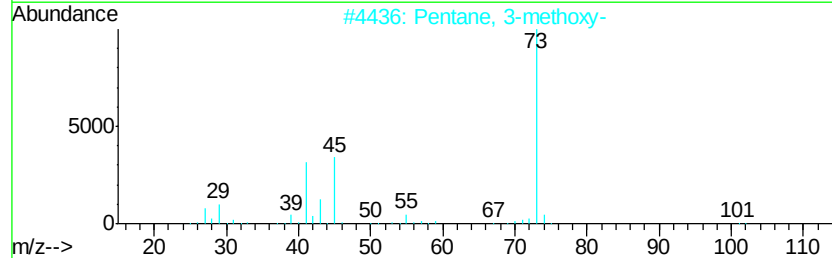
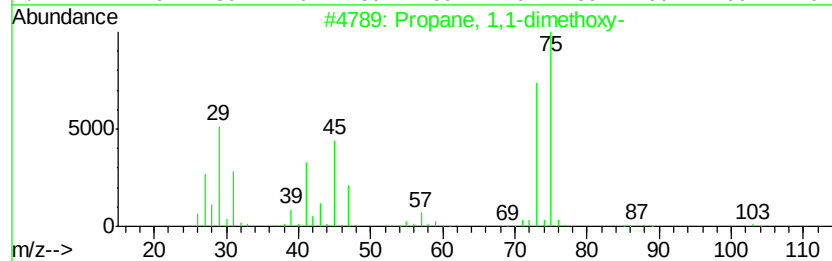
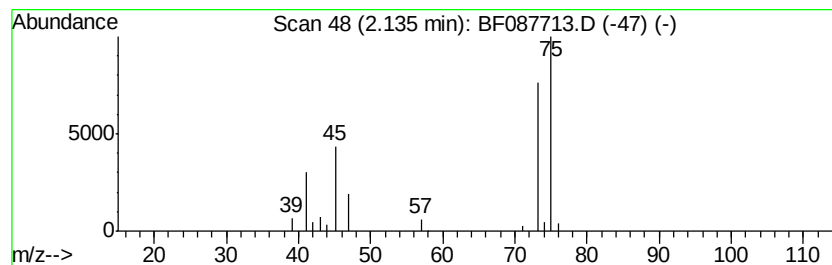
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.14	4.45 ng	198520	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	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
3		Glycine	75	C2H5NO2	000056-40-6	7
4		1,3-Dioxolane	74	C3H6O2	000646-06-0	4
5		Methane, nitroso-	45	CH3NO	000865-40-7	4



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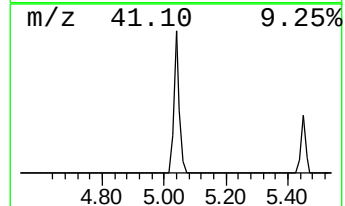
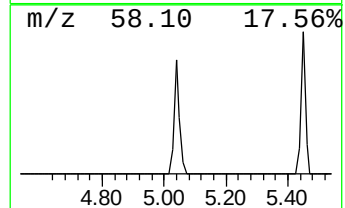
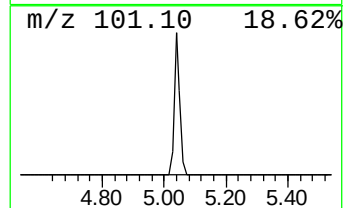
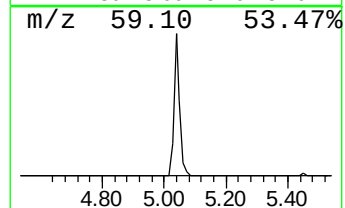
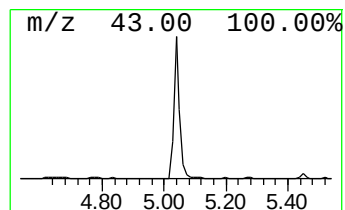
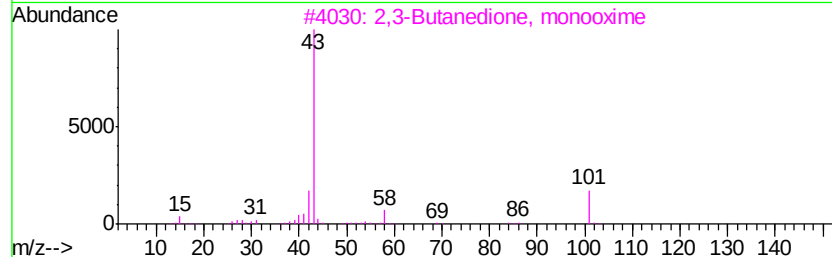
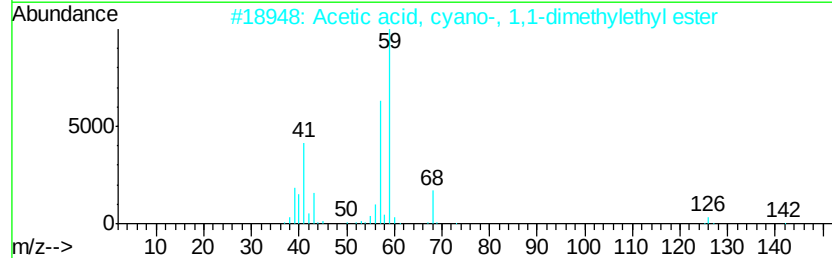
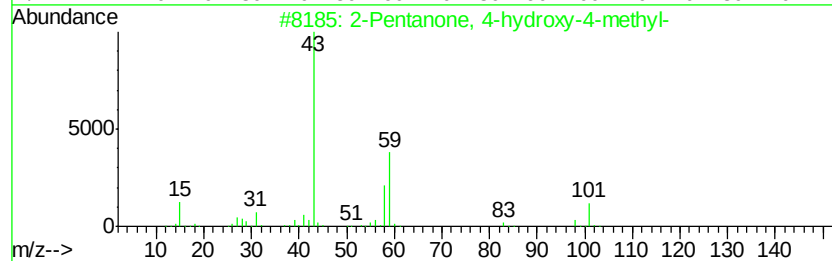
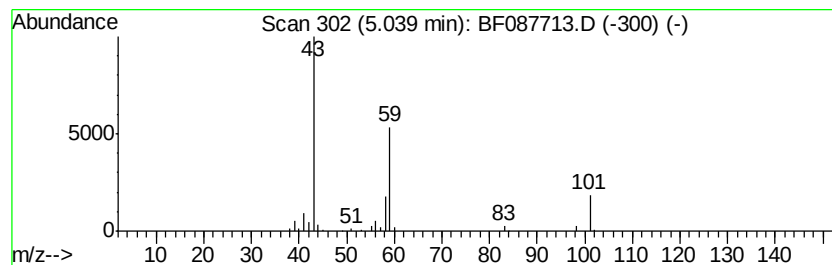
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	2.81 ng	125100	1,4-Dichlorobenzene-d4	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25		
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9		



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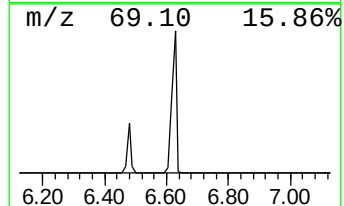
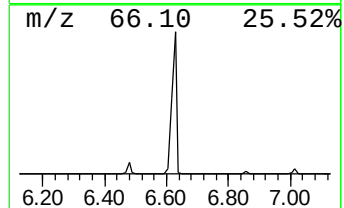
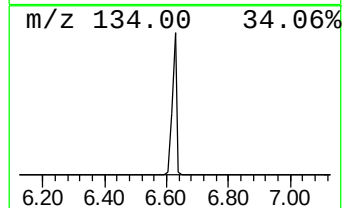
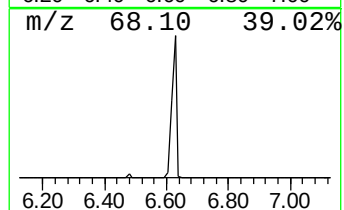
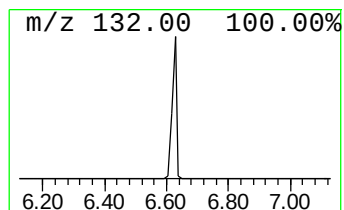
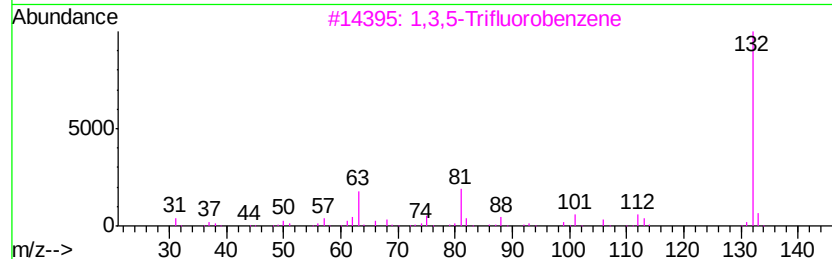
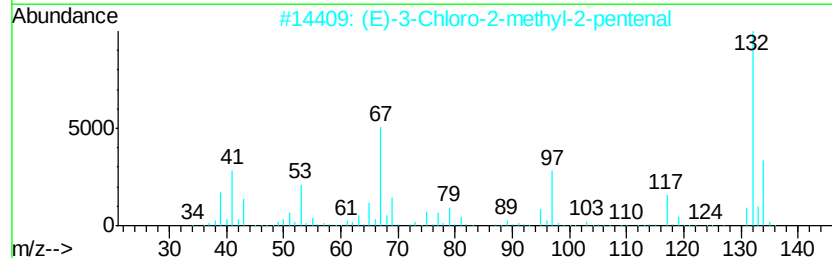
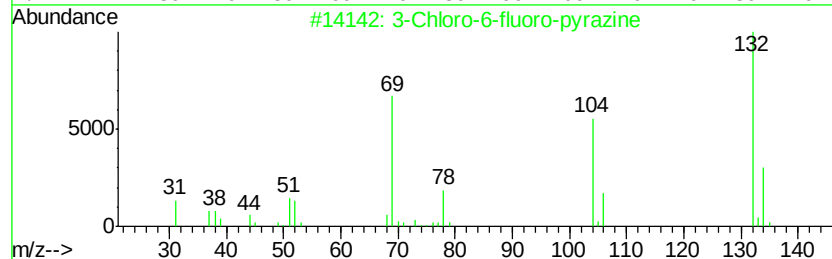
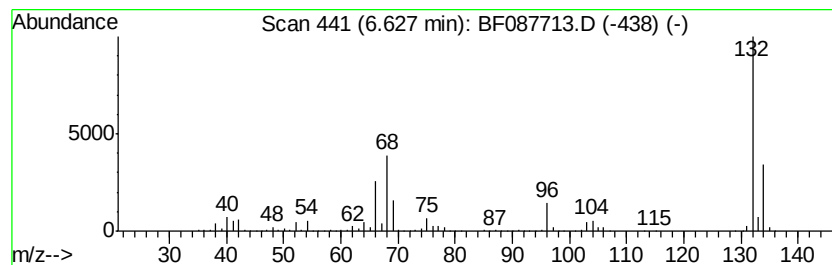
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Peak Number 5 unknown6.63 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.63	65.66 ng	2927430	1,4-Dichlorobenzene-d4	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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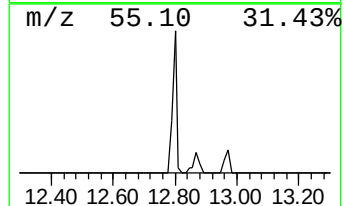
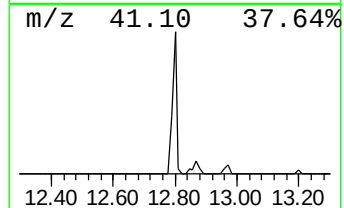
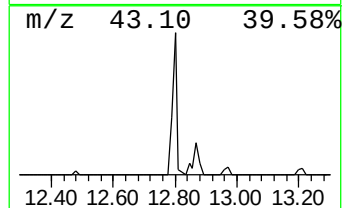
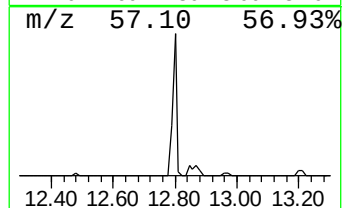
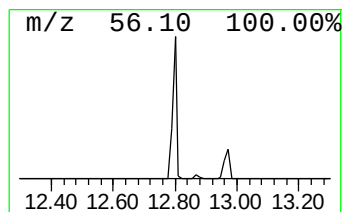
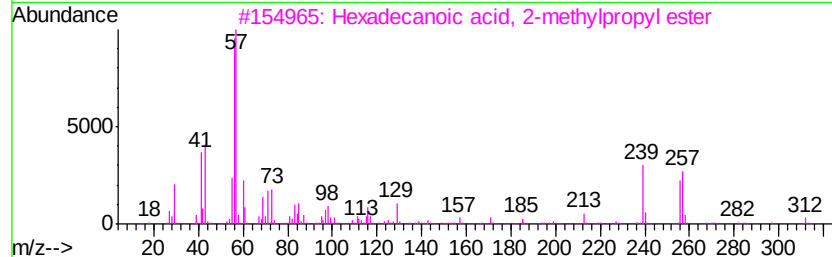
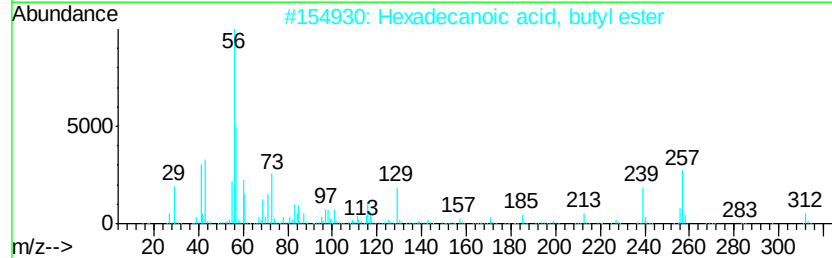
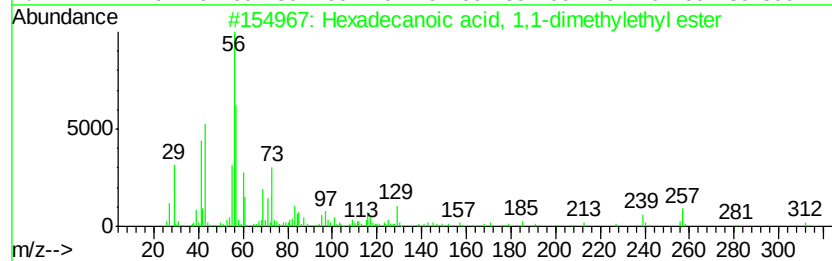
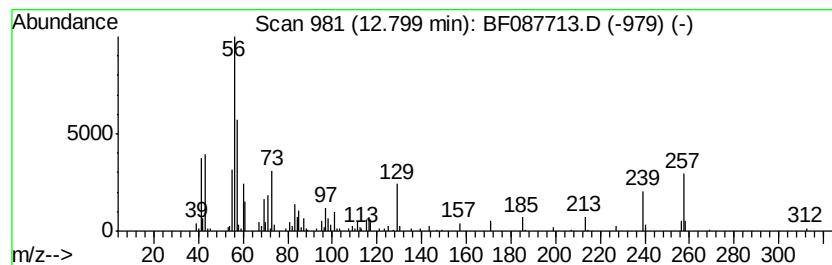
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.80	4.10 ng	233678	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2		Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	58
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		Butyl 4,8,12-trimethyl-tridecanoate	312	C20H40O2	1000336-63-2	42



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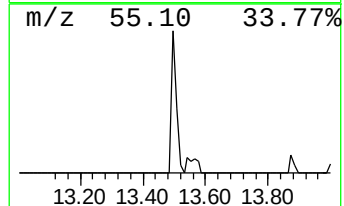
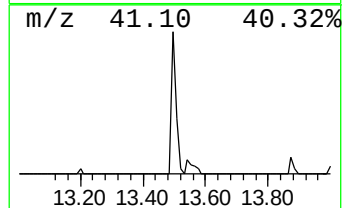
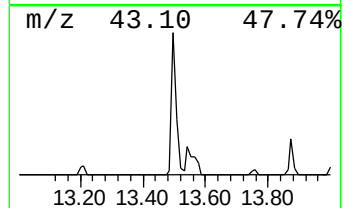
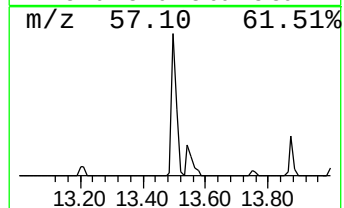
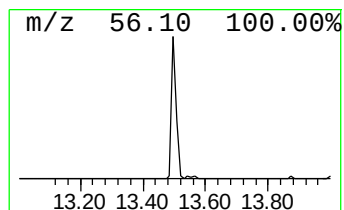
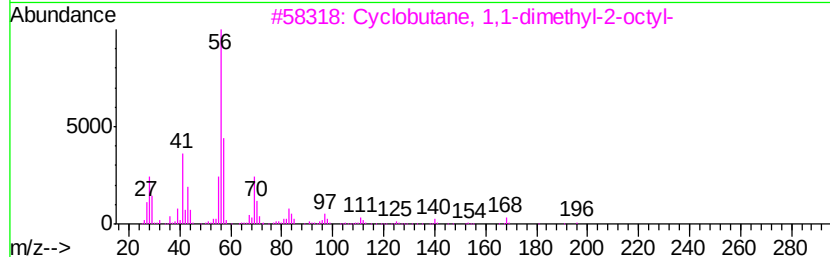
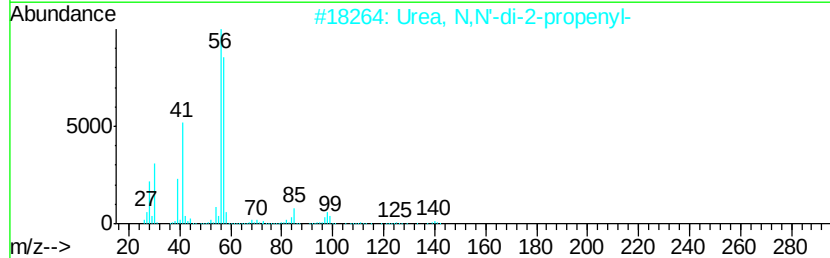
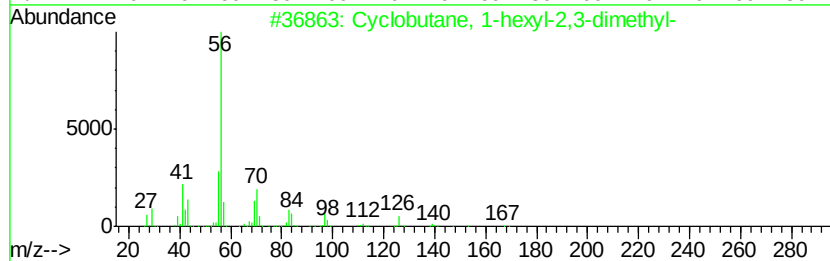
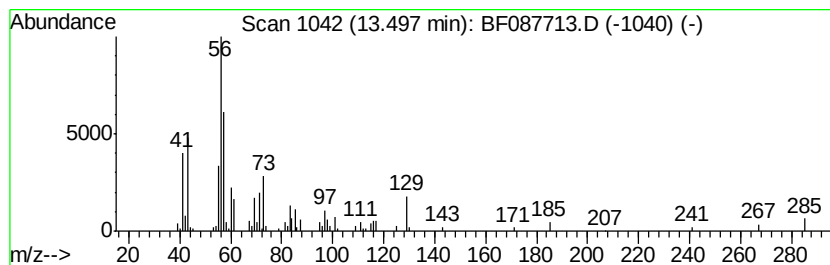
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Peak Number 8 unknown13.50 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.50	2.64 ng	150569	Chrysene-d12	14.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclobutane, 1-hexyl-2,3-dimethyl-	168	C12H24	055170-84-8	38
2		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	38
3		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	38
4		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	35
5		2-Methyl-1-octadecene	266	C19H38	061868-20-0	32



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Propane, 1,1-dime...	2.14	4.5	ng	198520	1	6.86	891657	20.0
2-Pentanone, 4-hy...	5.04	2.8	ng	125100	1	6.86	891657	20.0
unknown6.63	6.63	65.7	ng	2927430	1	6.86	891657	20.0
Hexadecanoic acid...	12.80	4.1	ng	233678	5	14.01	1140250	20.0
unknown13.50	13.50	2.6	ng	150569	5	14.01	1140250	20.0