

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040518\
 Data File : BF104294.D
 Acq On : 6 Apr 2018 2:16
 Operator : JU/SJ
 Sample : J2226-12
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 040318-SIDI-E-U-S

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-BF032818.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	2.246	22	27	43	rVB	352276	530988	11.79%	2.242%
2	5.169	521	524	537	rBV	41823	68657	1.52%	0.290%
3	5.598	591	597	622	rBV2	88752	548756	12.19%	2.317%
4	6.616	763	770	784	rBV2	86517	437974	9.73%	1.849%
5	6.716	784	787	824	rVV	936235	2165691	48.10%	9.142%
6	6.951	824	827	848	rVV	159991	641310	14.24%	2.707%
7	7.098	848	852	897	rVB	1864758	2917844	64.80%	12.317%
8	7.516	919	923	944	rBV	927675	2029548	45.08%	8.568%
9	8.228	1040	1044	1069	rBV	337303	791282	17.57%	3.340%
10	9.298	1222	1226	1261	rBV	3054621	4502570	100.00%	19.007%
11	9.981	1339	1342	1362	rBV	733155	931281	20.68%	3.931%
12	10.775	1474	1477	1489	rBV	1070837	1699471	37.74%	7.174%
13	10.857	1489	1491	1502	rVB	75385	136127	3.02%	0.575%
14	11.480	1593	1597	1619	rBV	531936	974162	21.64%	4.112%
15	13.063	1861	1866	1889	rBV	2946026	3815810	84.75%	16.108%
16	13.927	2009	2013	2027	rBV	86448	131102	2.91%	0.553%
17	14.133	2044	2048	2065	rBV	467917	784422	17.42%	3.311%
18	15.663	2303	2308	2331	rBV	259649	581653	12.92%	2.455%

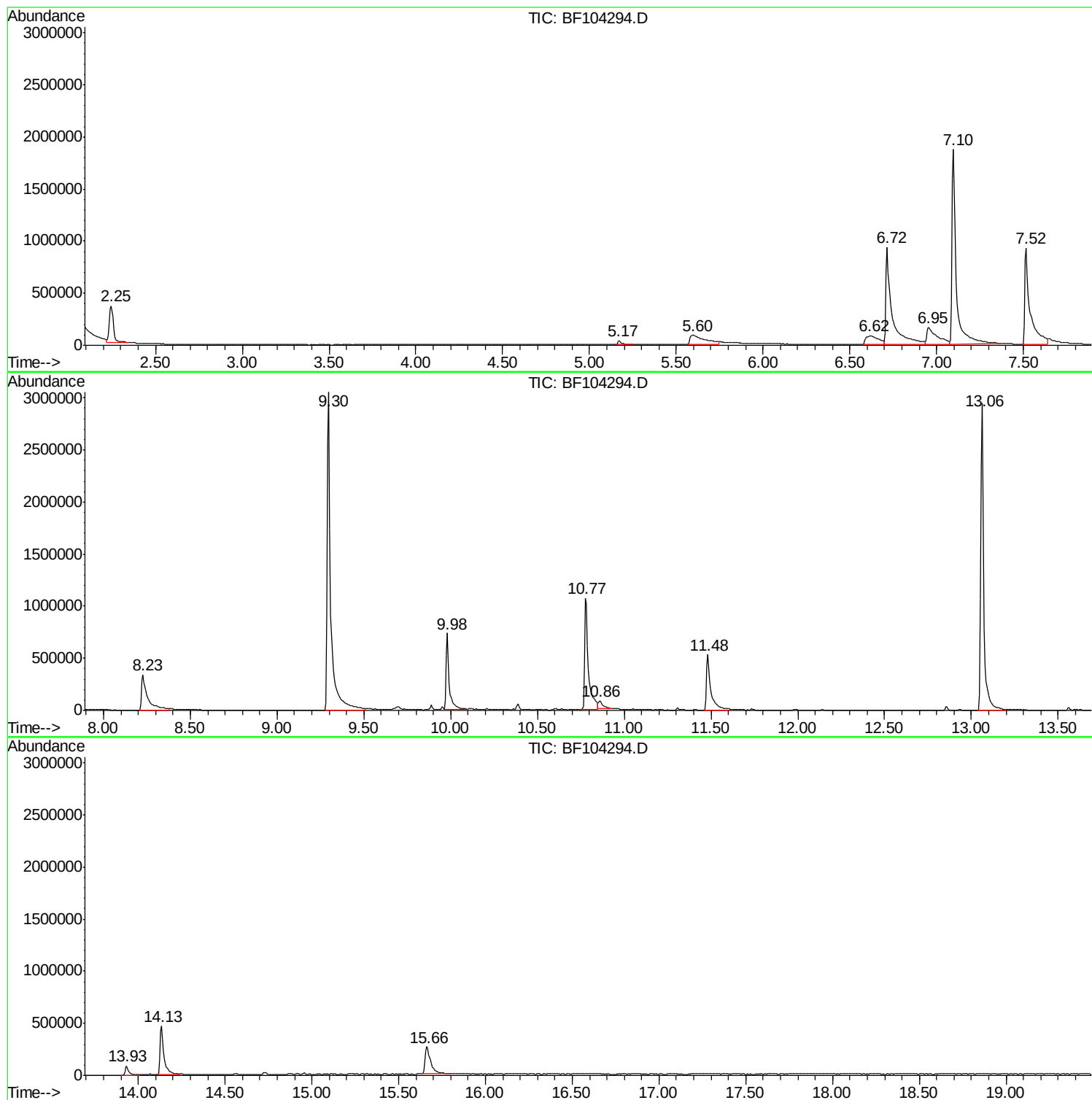
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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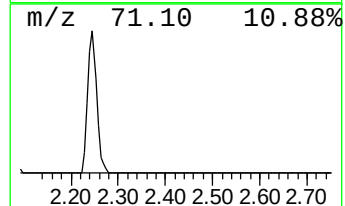
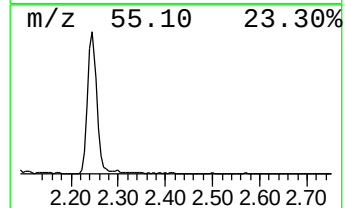
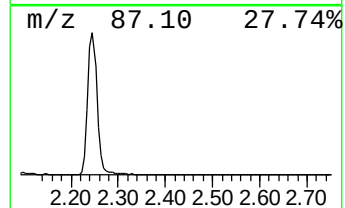
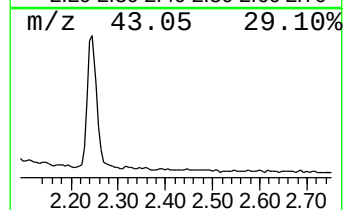
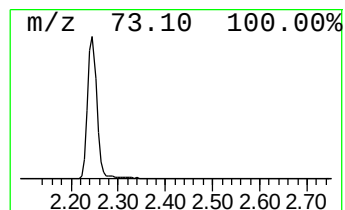
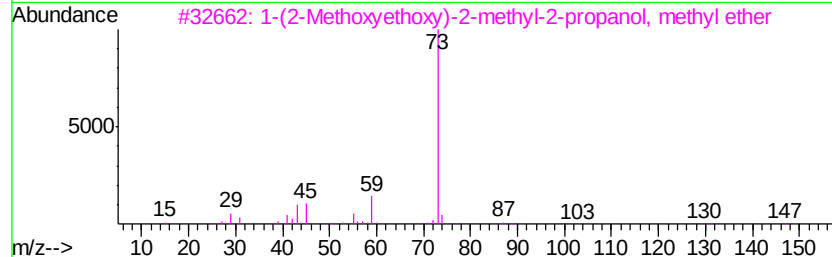
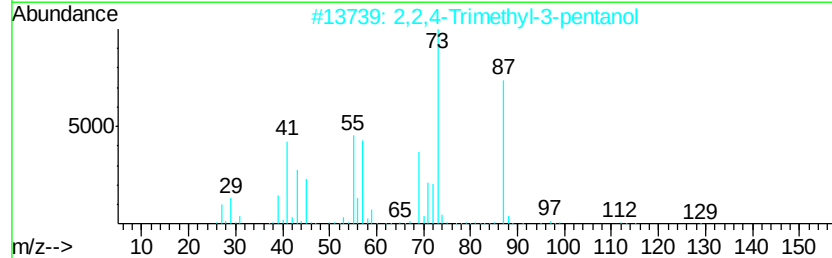
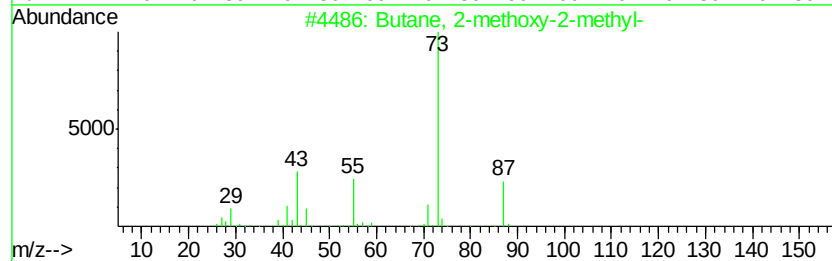
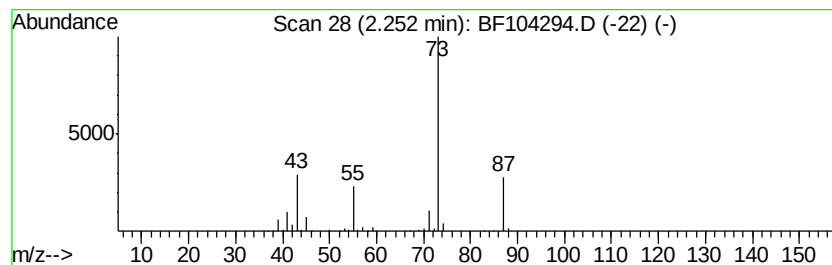
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.25	16.56 ng	530988	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1-(2-Methoxyethoxy)-2-methyl-2-propanol	162	C8H18O3	1000364-24-4	25
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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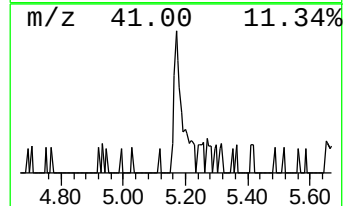
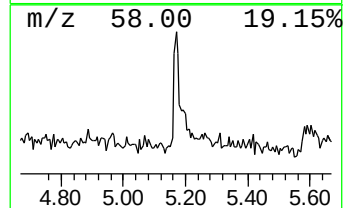
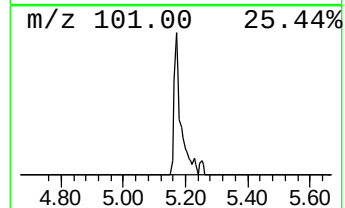
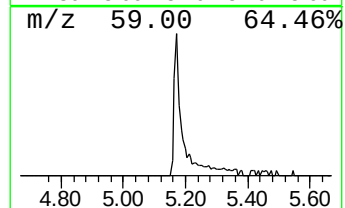
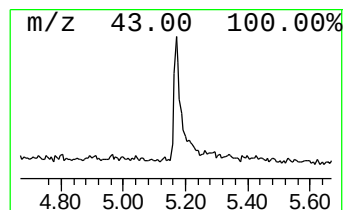
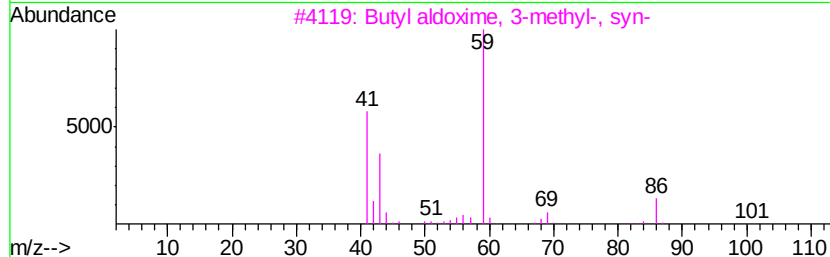
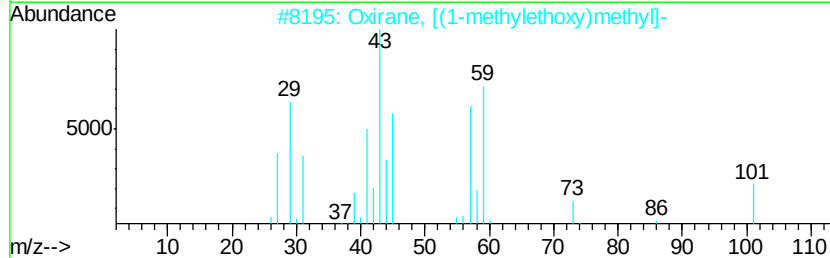
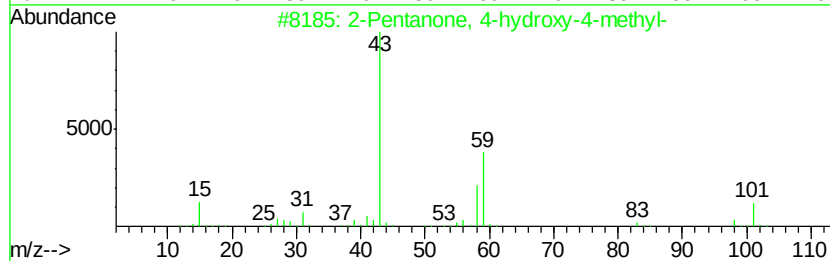
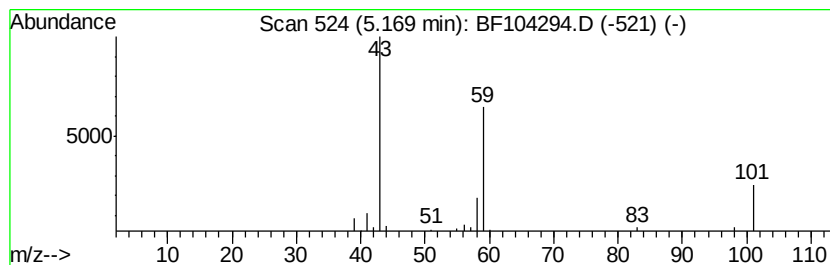
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	2.14 ng	68657	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	38
3			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	16
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	12
5			5-Hexen-2-one	98	C6H10O	000109-49-9	10



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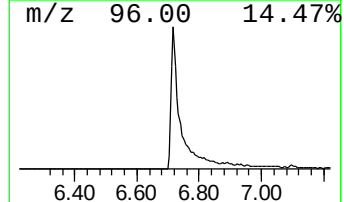
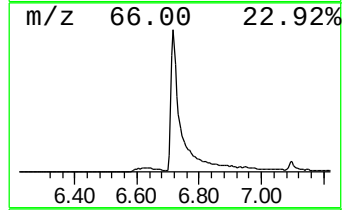
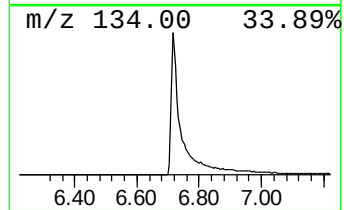
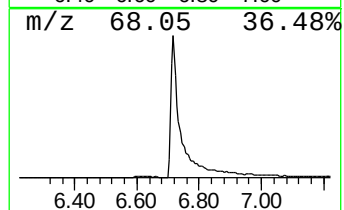
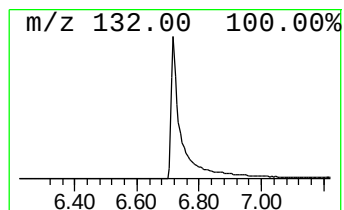
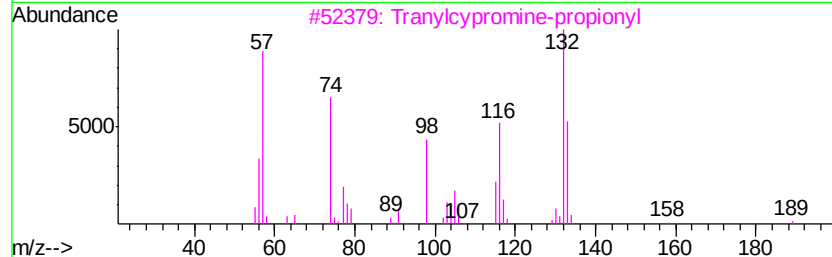
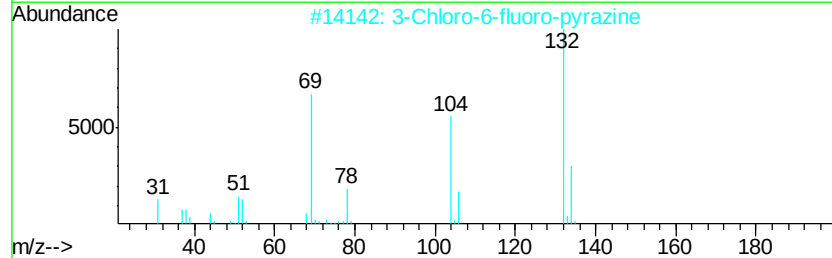
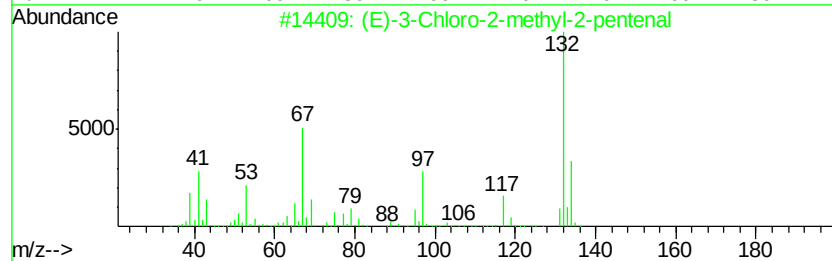
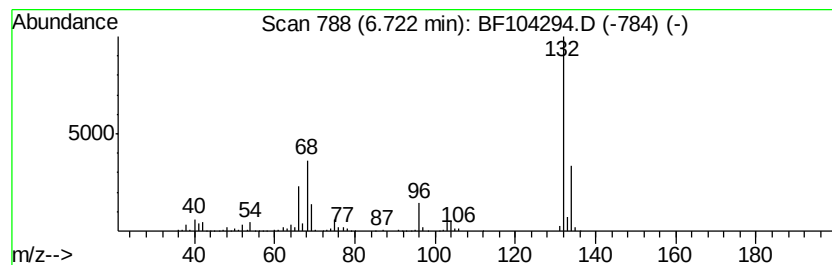
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Peak Number 3 unknown6.72 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	67.54 ng	2165690	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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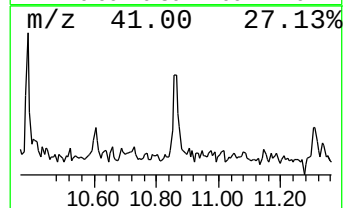
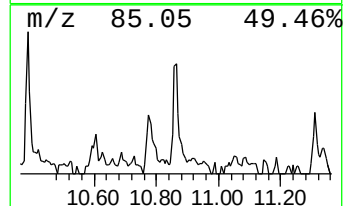
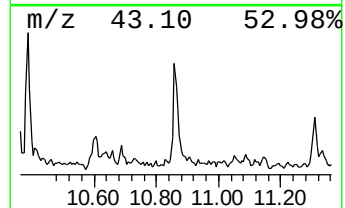
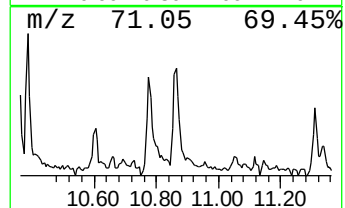
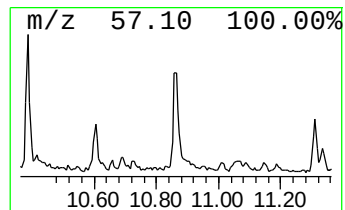
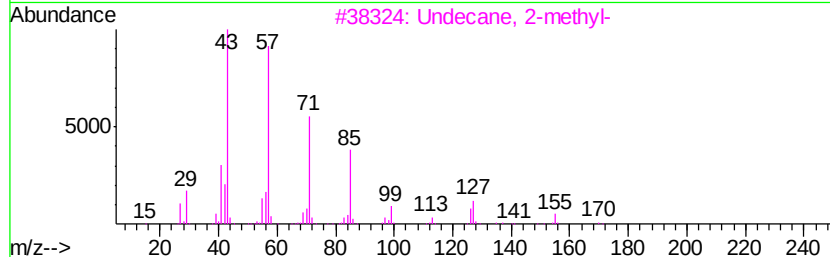
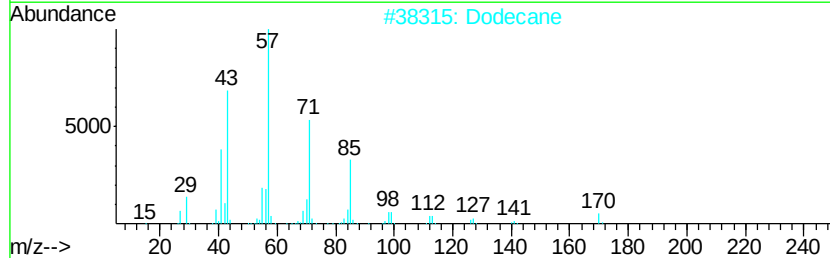
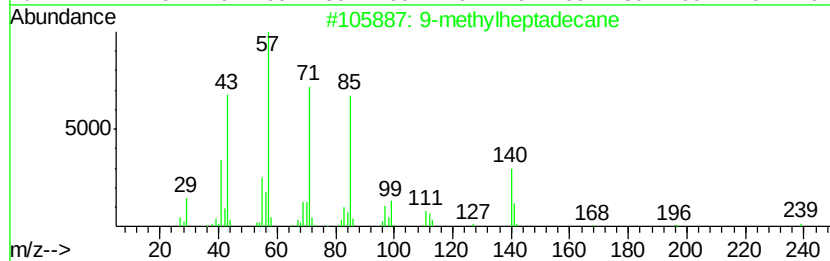
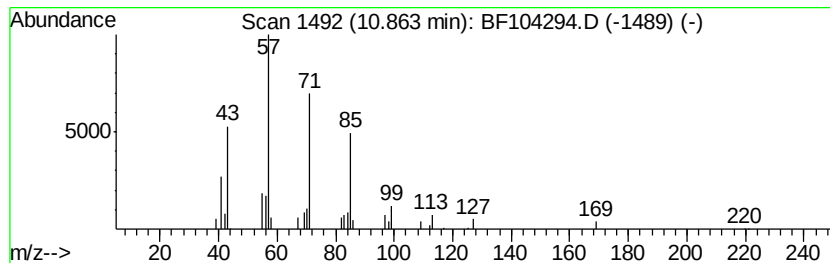
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Peak Number 5 9-methylheptadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.86	2.79 ng	136127	Phenanthrene-d10	11.48	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-methylheptadecane	254	C18H38	026741-18-4	86
2	Dodecane	170	C12H26	000112-40-3	81
3	Undecane, 2-methyl-	170	C12H26	007045-71-8	80
4	Tetradecane	198	C14H30	000629-59-4	80
5	Pentadecane	212	C15H32	000629-62-9	80



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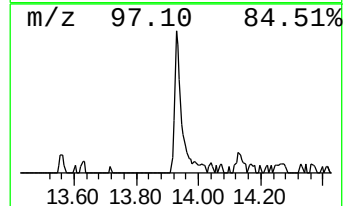
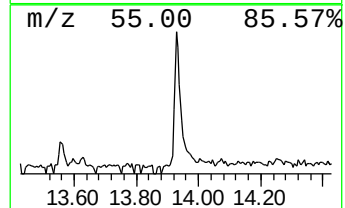
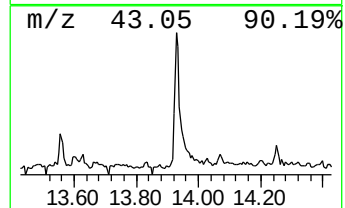
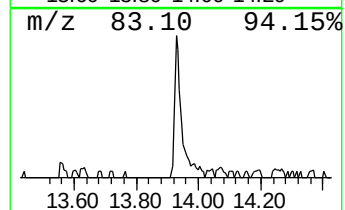
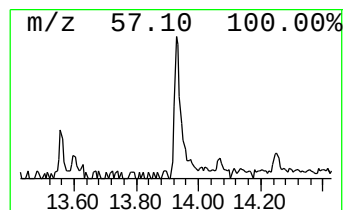
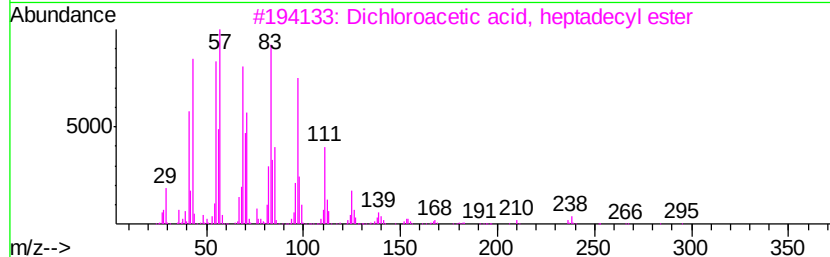
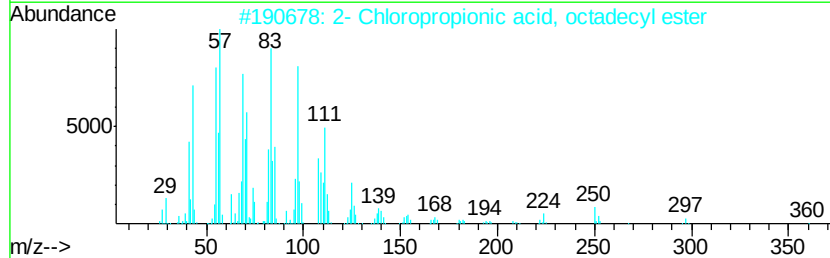
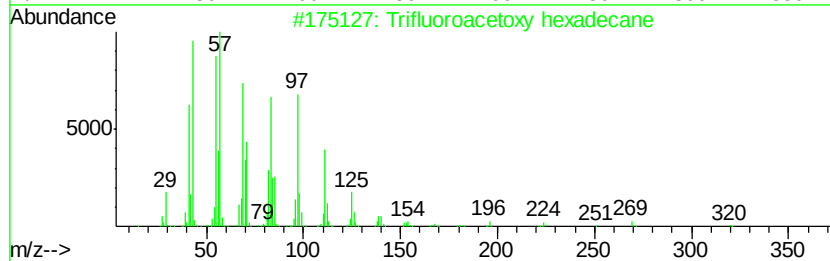
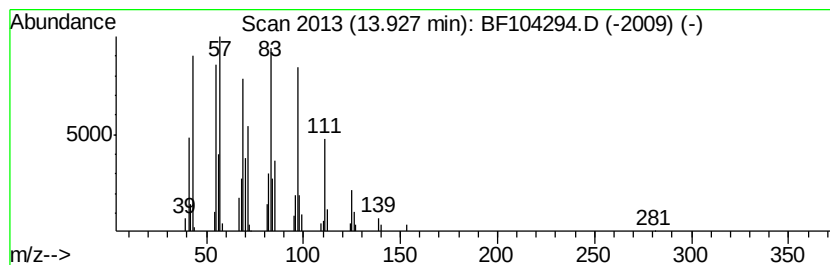
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.93	3.34 ng	131102	Chrysene-d12	14.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
2		2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
3		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
4		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
5		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	92



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.25	16.6	ng	530988	1	6.95	641310	20.0
2-Pentanone, 4-hy...	5.17	2.1	ng	68657	1	6.95	641310	20.0
unknown6.72	6.72	67.5	ng	2165690	1	6.95	641310	20.0
9-methylheptadecane	10.86	2.8	ng	136127	4	11.48	974162	20.0
Trifluoroacetoxy ...	13.93	3.3	ng	131102	5	14.13	784422	20.0