

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081718\
 Data File : BF108269.D
 Acq On : 18 Aug 2018 3:42
 Operator : JU/SJ
 Sample : J4511-02
 Misc :
 ALS Vial : 37 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RA-081418-FL-024

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF080818.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	2.372	3	6	14	rVB	455388	581631	10.26%	1.352%
2	3.672	225	227	241	rBV	38747	85678	1.51%	0.199%
3	5.272	495	499	506	rBV	185262	247660	4.37%	0.576%
4	5.654	558	564	567	rBV	4439700	4715698	83.15%	10.963%
5	6.642	726	732	735	rBV	4351068	5089799	89.75%	11.832%
6	6.790	752	757	760	rBV	4860465	4928215	86.90%	11.457%
7	7.013	792	795	799	rBV	1092289	984967	17.37%	2.290%
8	7.172	818	822	826	rBV	3917188	3847516	67.84%	8.944%
9	7.584	886	892	895	rBV	2990313	3316423	58.48%	7.710%
10	8.301	1010	1014	1017	rBV	1366193	1192163	21.02%	2.771%
11	9.372	1191	1196	1200	rBV	5525337	5671254	100.00%	13.184%
12	9.760	1259	1262	1267	rBV	404644	339132	5.98%	0.788%
13	10.060	1309	1313	1317	rBV2	1498275	1274929	22.48%	2.964%
14	10.854	1444	1448	1460	rBV	2996605	2926926	51.61%	6.804%
15	11.554	1564	1567	1571	rBV	1155021	1094489	19.30%	2.544%
16	13.148	1833	1838	1841	rBV	4453220	4241778	74.79%	9.861%
17	14.054	1988	1992	2004	rBV2	112722	236072	4.16%	0.549%
18	14.213	2015	2019	2030	rVB	1200244	1098612	19.37%	2.554%
19	14.977	2145	2149	2151	rBV2	51711	62358	1.10%	0.145%
20	15.060	2161	2163	2169	rVB	70333	78064	1.38%	0.181%
21	15.342	2208	2211	2217	rVB	54310	61298	1.08%	0.142%
22	15.777	2278	2285	2298	rVB	565623	865953	15.27%	2.013%
23	16.236	2359	2363	2366	rBV2	41955	75567	1.33%	0.176%

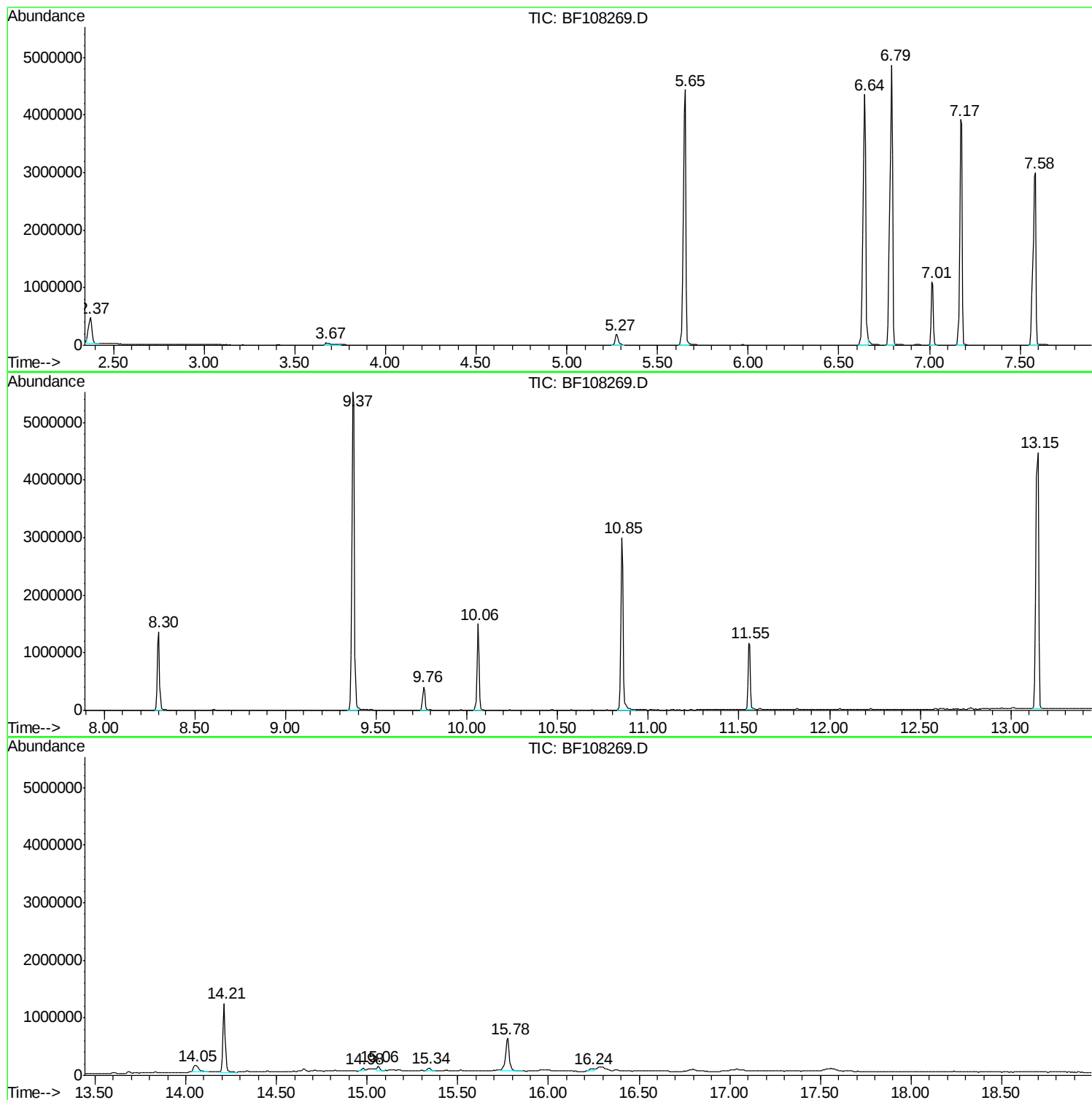
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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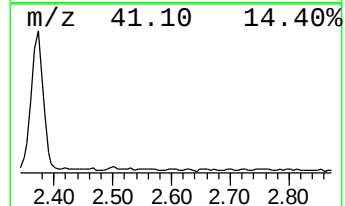
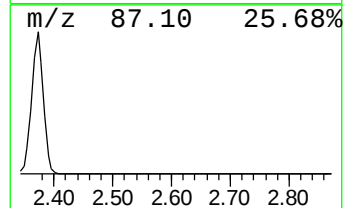
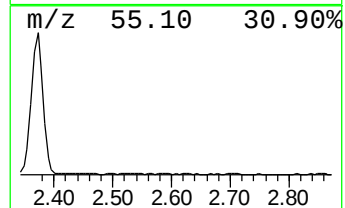
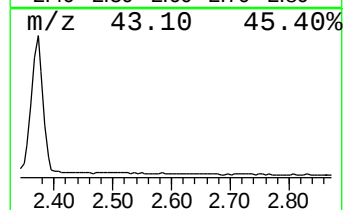
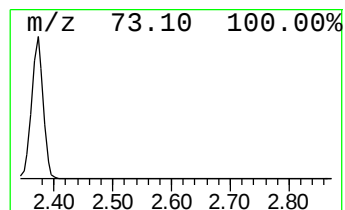
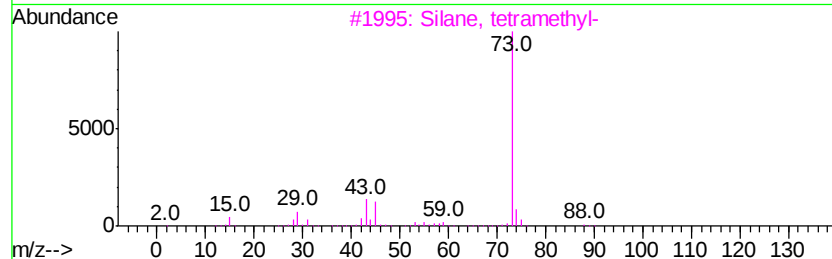
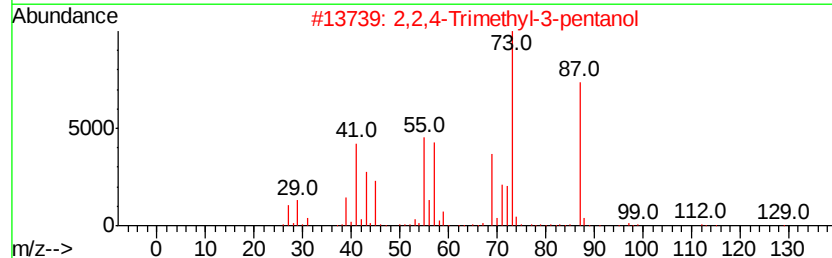
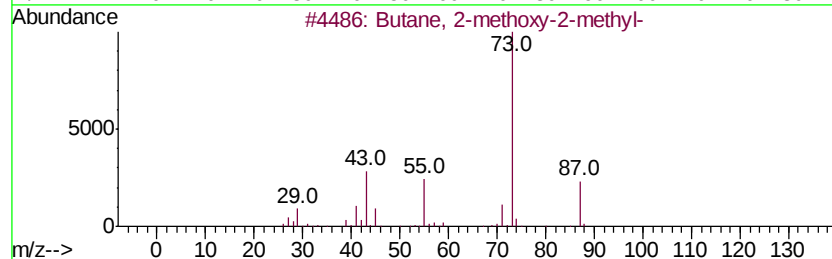
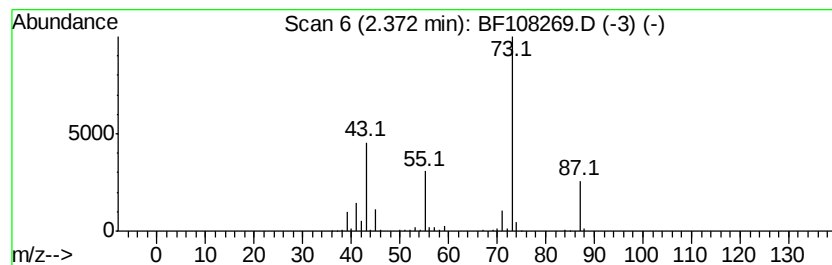
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF080818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.37	11.81 ng	581631	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	32



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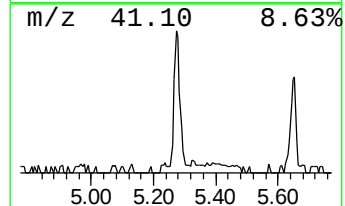
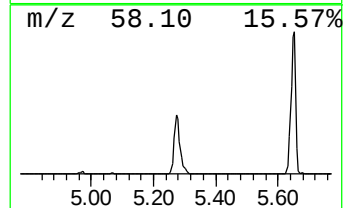
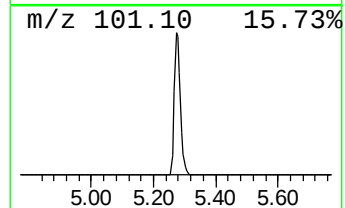
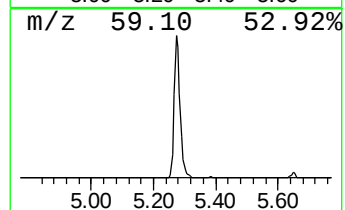
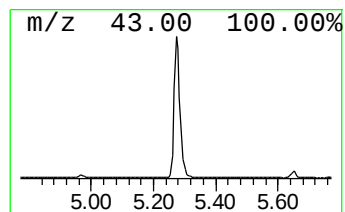
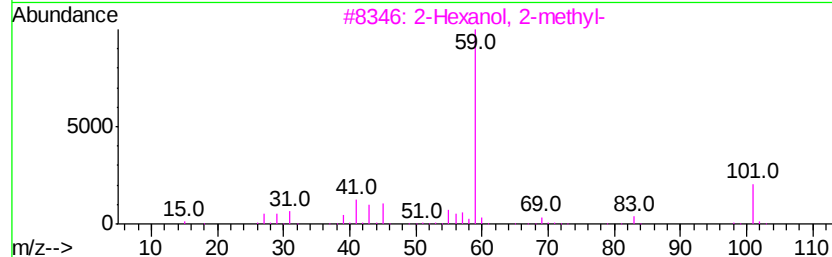
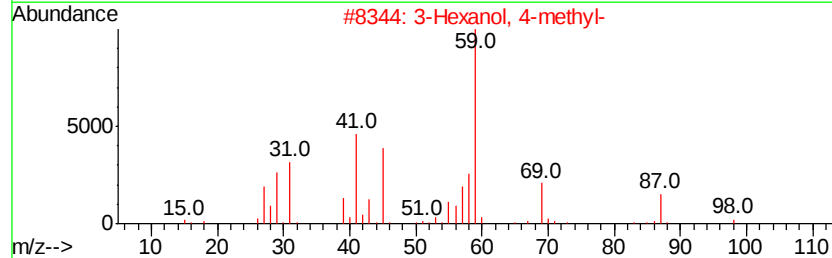
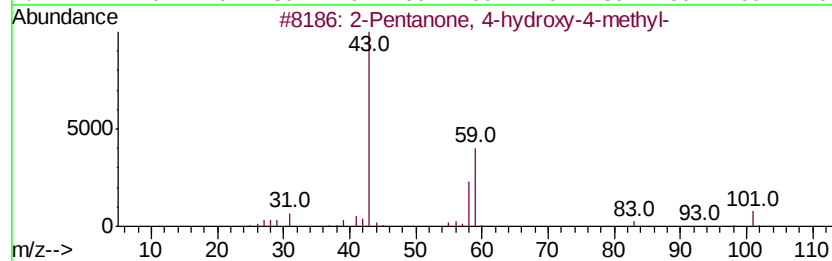
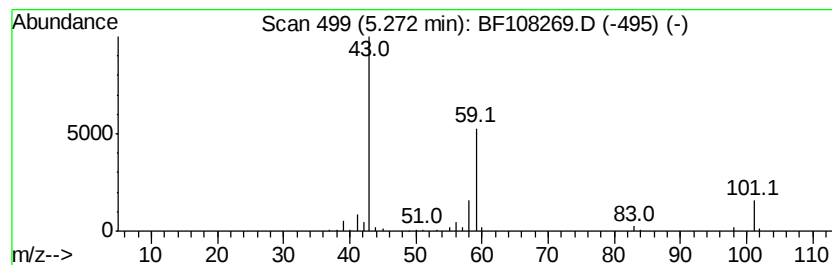
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.27	5.03 ng	247660	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
5		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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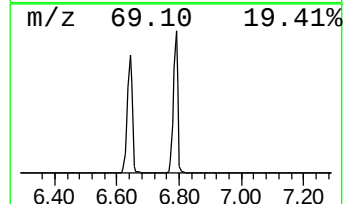
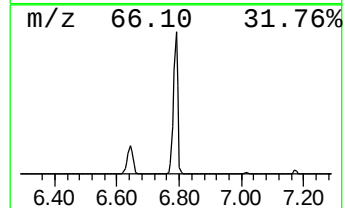
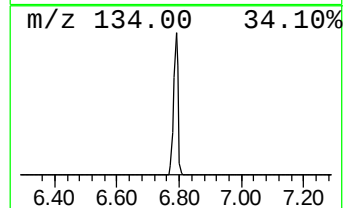
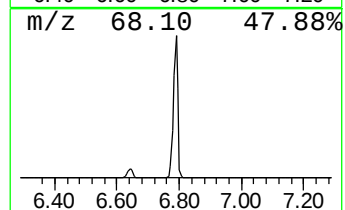
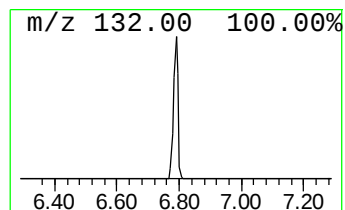
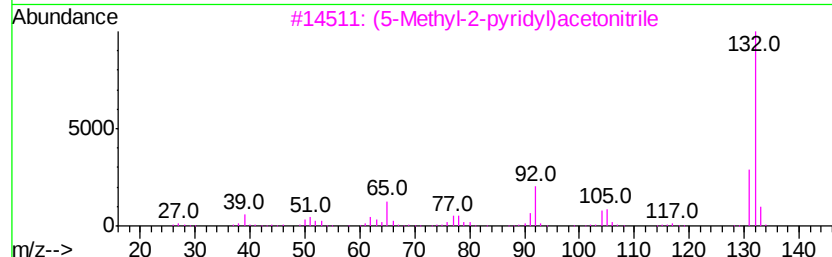
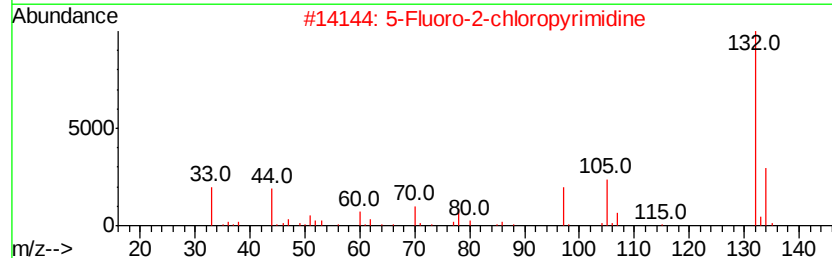
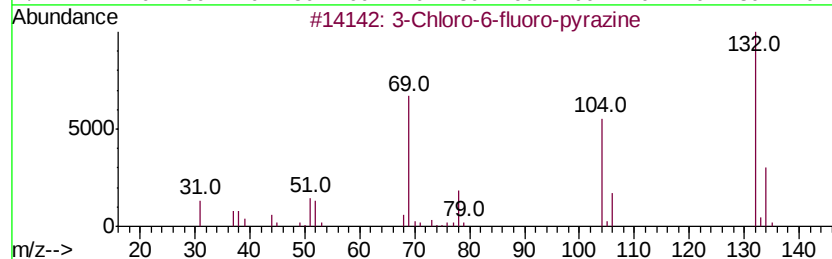
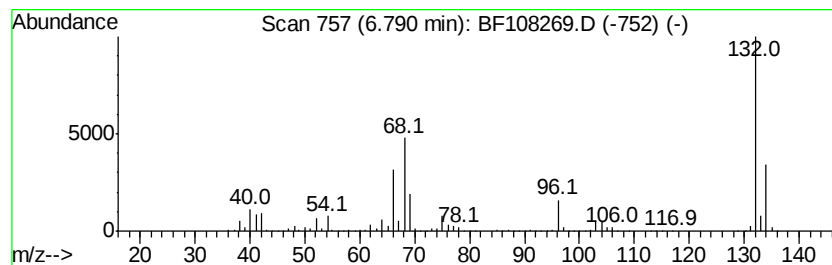
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Peak Number 3 unknown6.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.79	100.07 ng	4928220	1,4-Dichlorobenzene-d4	7.02

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-Methyl-2-pyridyl)acetonitrile	132	C8H8N2	1000241-93-9	10
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	9



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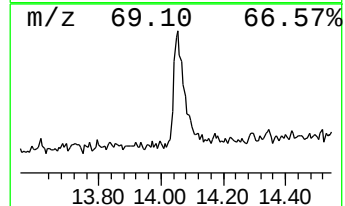
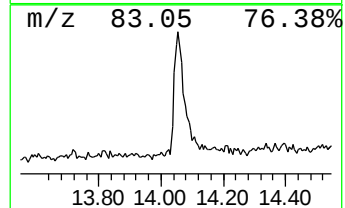
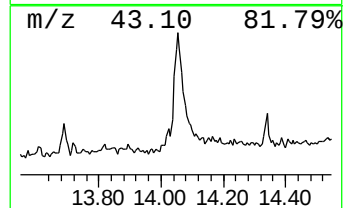
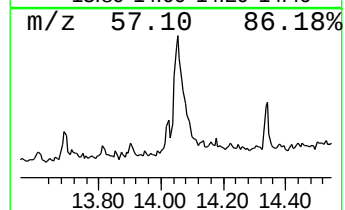
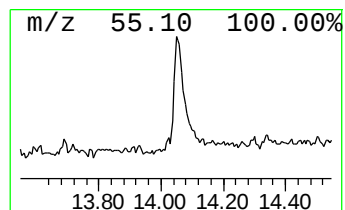
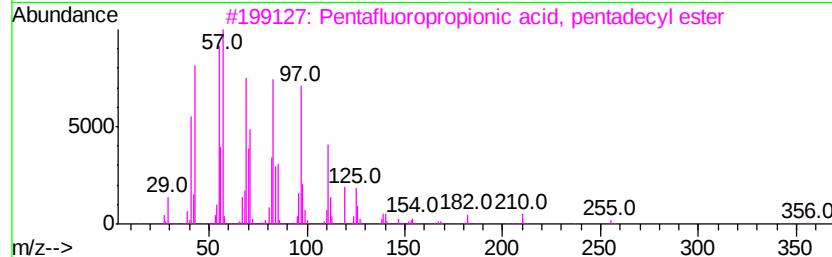
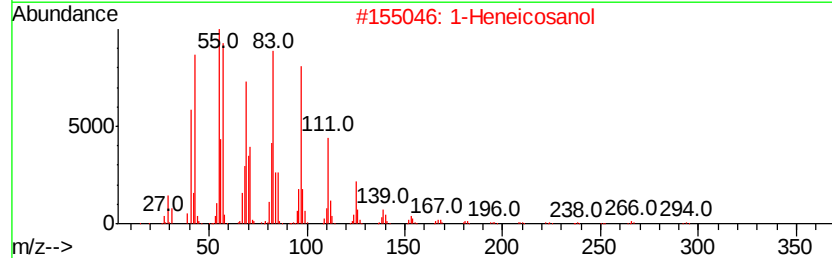
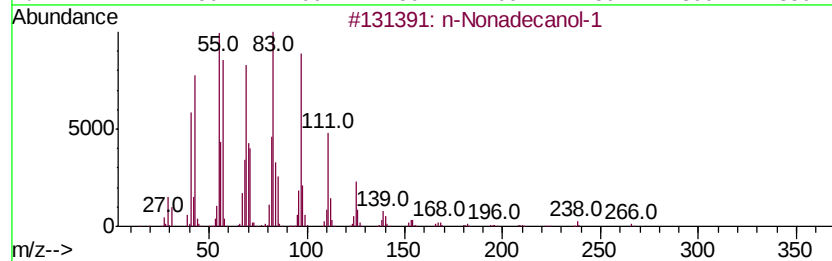
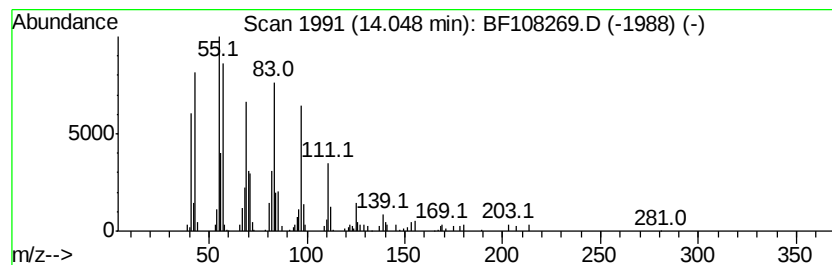
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Peak Number 5 n-Nonadecanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.05	4.30 ng	236072	Chrysene-d12	14.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1	284	C19H40O	001454-84-8	95	
2	1-Heneicosanol	312	C21H44O	015594-90-8	94	
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93	
4	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93	
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93	



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.37	11.8	ng	581631	1	7.02	984967	20.0
2-Pentanone, 4-hy...	5.27	5.0	ng	247660	1	7.02	984967	20.0
unknown6.79	6.79	100.1	ng	4928220	1	7.02	984967	20.0
n-Nonadecanol-1	14.05	4.3	ng	236072	5	14.21	1098610	20.0