

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF111519\
 Data File : BF117822.D
 Acq On : 16 Nov 2019 00:02
 Operator : JU
 Sample : K5861-18
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 EP-15

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF111319.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	2.175	10	15	33	rVB	853356	1240829	16.28%	2.106%
2	5.128	509	517	526	rBV	970956	1211049	15.89%	2.056%
3	5.528	580	585	588	rBV	5240158	5435559	71.32%	9.227%
4	6.539	751	757	761	rBV	5489066	5680424	74.54%	9.643%
5	6.686	777	782	785	rBV	6122612	5718950	75.04%	9.708%
6	6.916	818	821	825	rBV	1529391	1272766	16.70%	2.161%
7	7.075	844	848	851	rBV	5246272	4574735	60.03%	7.766%
8	7.481	912	917	920	rBV	4002994	3548577	46.56%	6.024%
9	8.204	1036	1040	1044	rBV	2086048	1640822	21.53%	2.785%
10	9.286	1219	1224	1227	rBV	7449066	6713657	88.09%	11.397%
11	9.675	1287	1290	1294	rBV	923105	690957	9.07%	1.173%
12	9.969	1336	1340	1343	rBV	2320707	1936762	25.41%	3.288%
13	10.757	1470	1474	1477	rBV	5016358	4540869	59.58%	7.708%
14	11.457	1589	1593	1597	rBV	2294418	2090822	27.44%	3.549%
15	11.980	1679	1682	1694	rBV	396652	418189	5.49%	0.710%
16	12.768	1813	1816	1830	rBV2	89835	126311	1.66%	0.214%
17	13.051	1859	1864	1867	rBV	8033425	7620953	100.00%	12.937%
18	13.957	2011	2018	2038	rBV4	130671	532736	6.99%	0.904%
19	14.104	2039	2043	2047	rVB	2203959	1908456	25.04%	3.240%
20	14.974	2187	2191	2195	rVB	94202	89360	1.17%	0.152%
21	15.609	2293	2299	2304	rBV	1468116	1915194	25.13%	3.251%

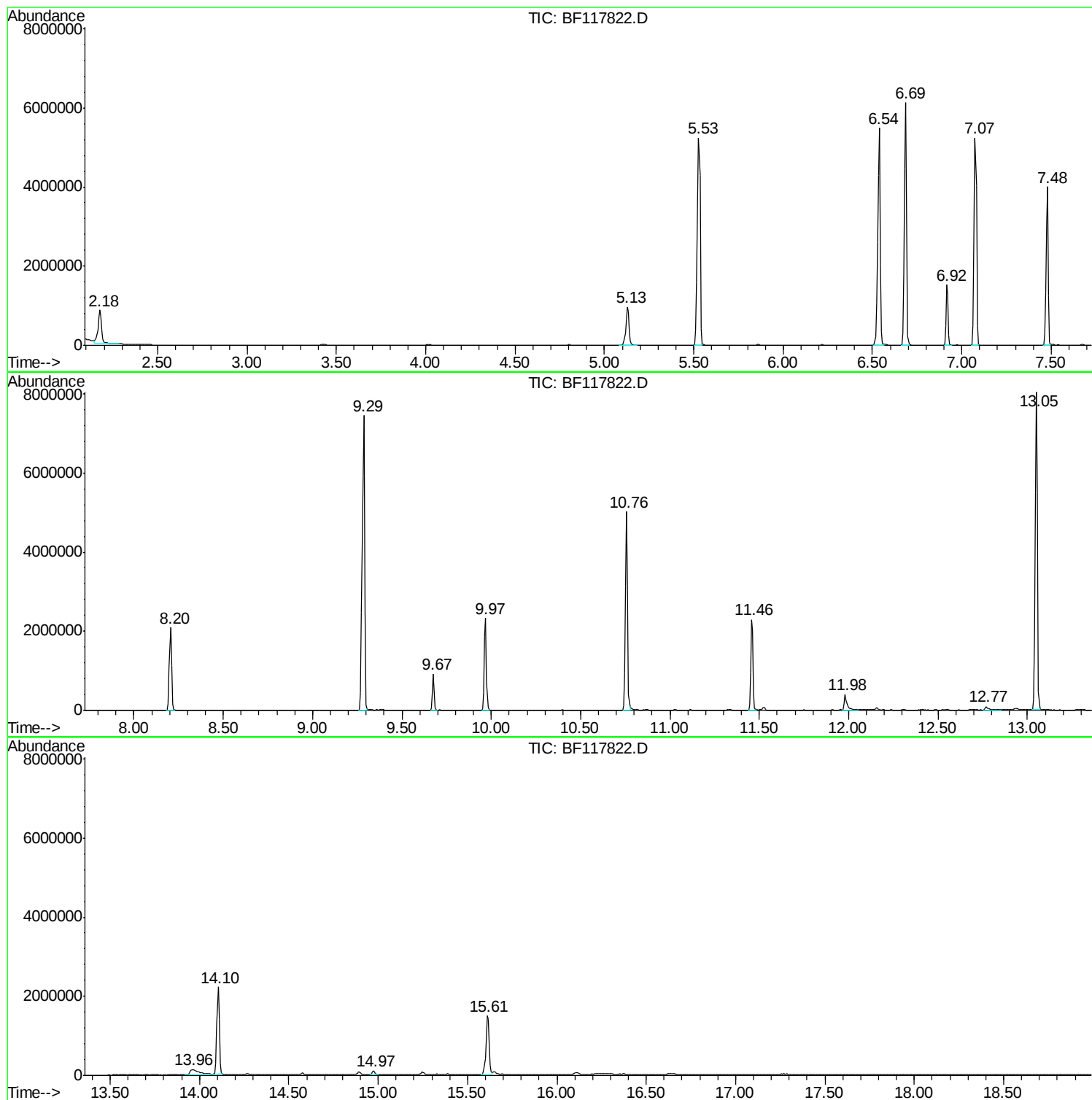
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF111319.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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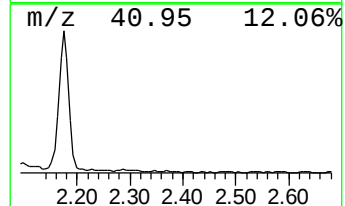
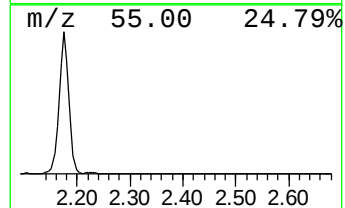
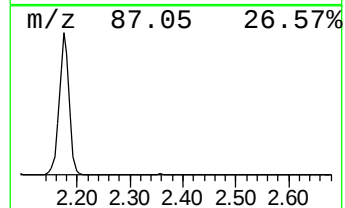
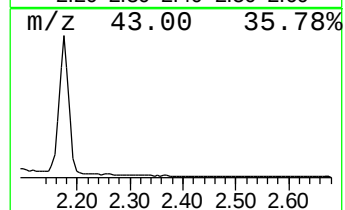
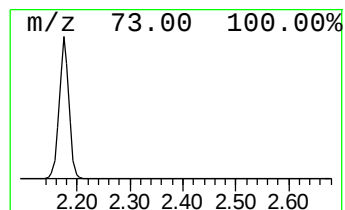
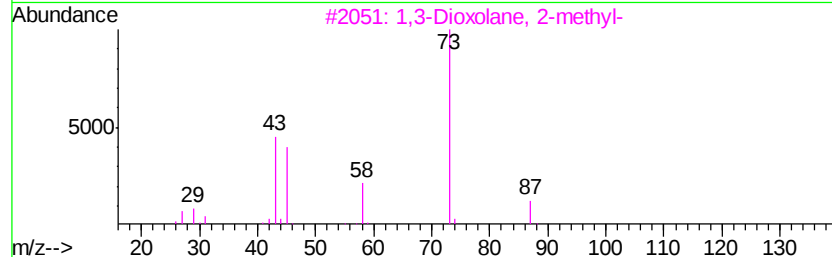
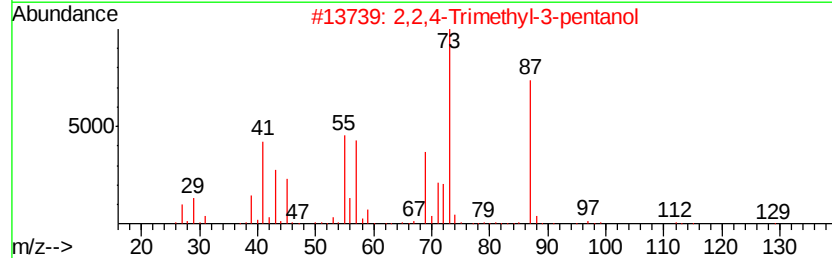
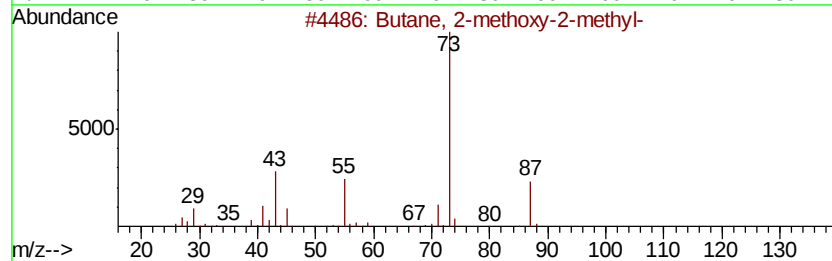
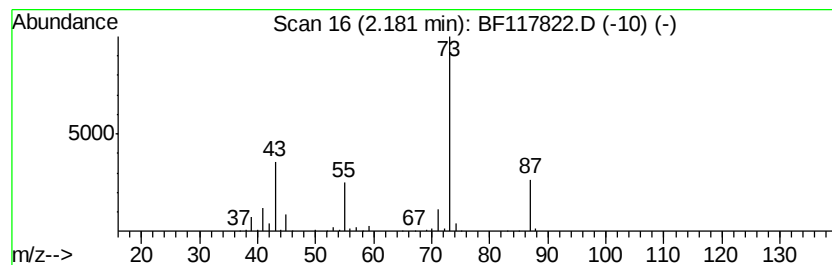
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	19.50 ng	1240830	1,4-Dichlorobenzene-d4	6.92

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		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10



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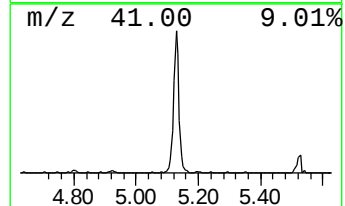
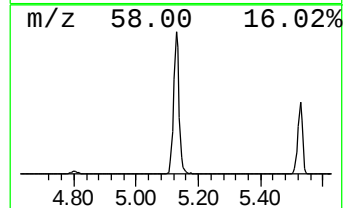
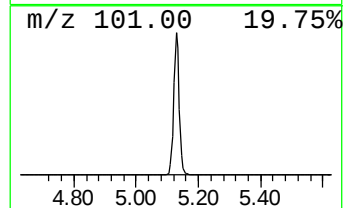
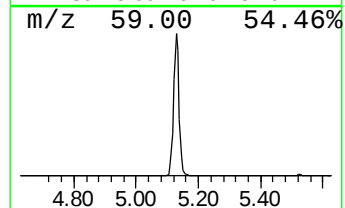
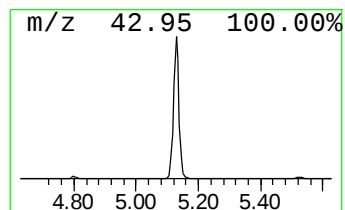
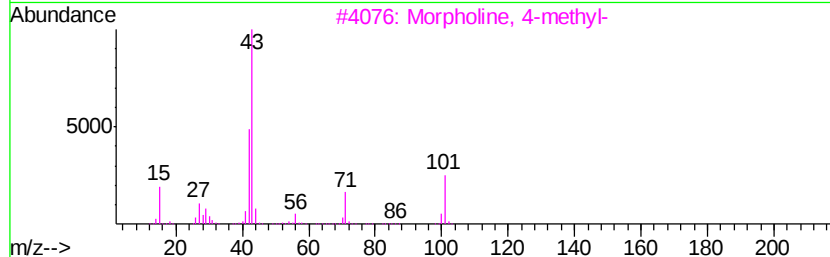
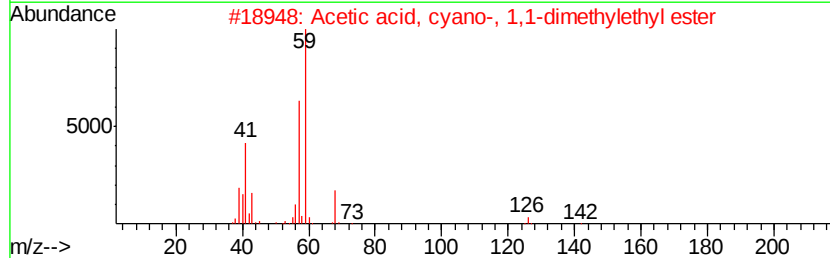
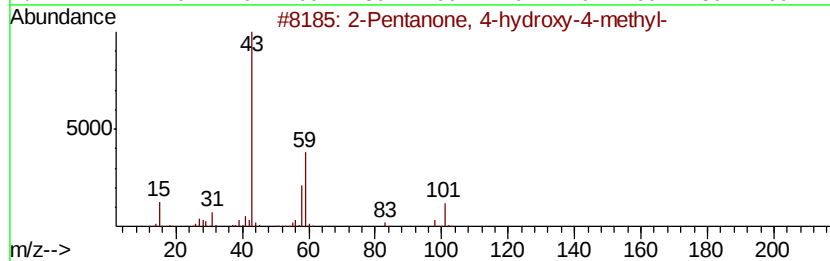
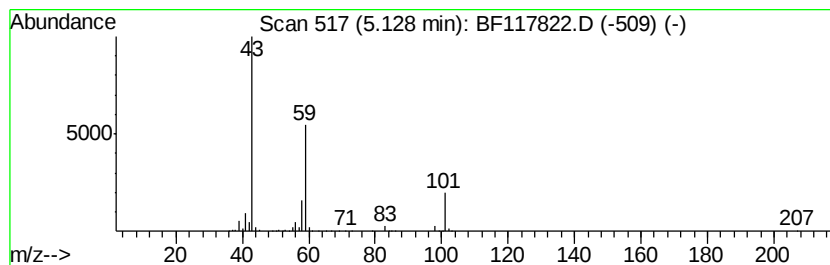
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	19.03 ng	1211050	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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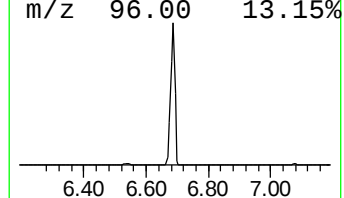
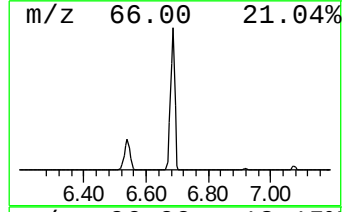
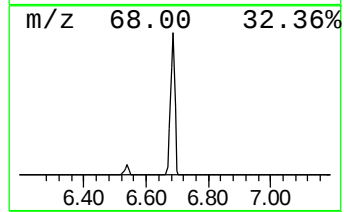
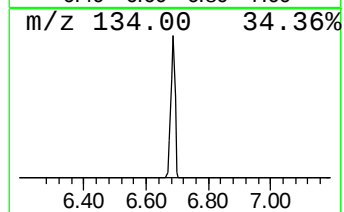
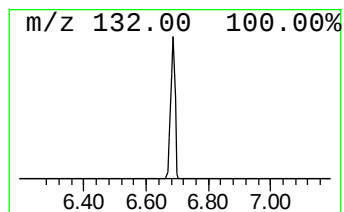
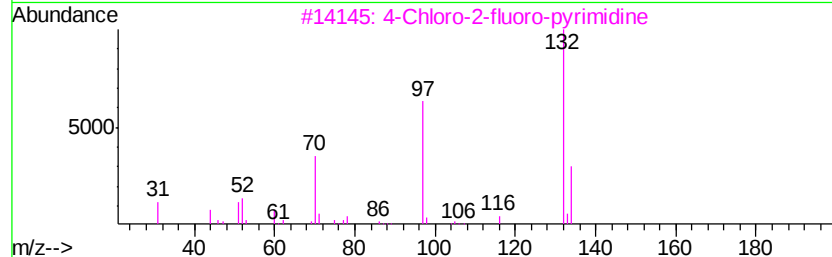
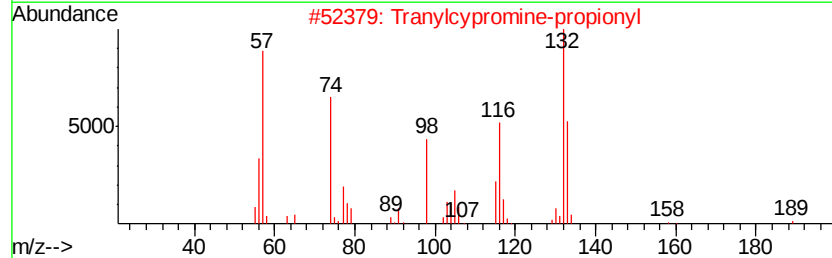
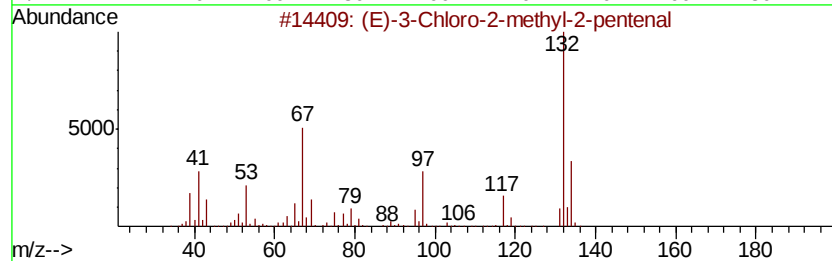
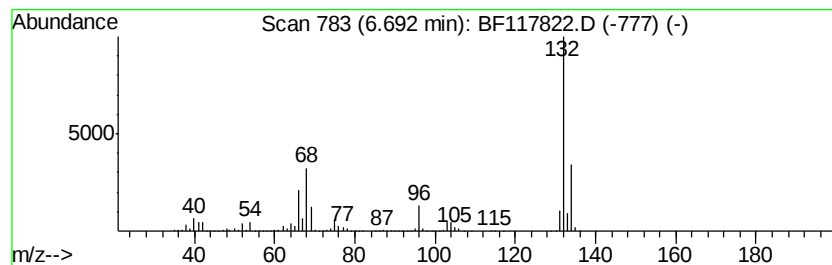
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Peak Number 3 unknown6.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.69	89.87 ng	5718950	1,4-Dichlorobenzene-d4	6.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
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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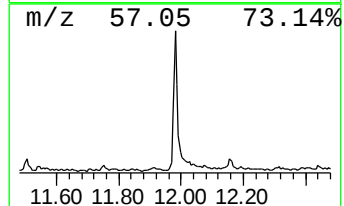
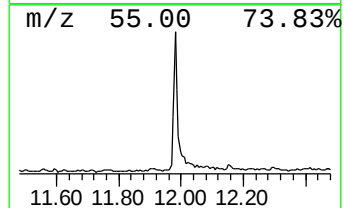
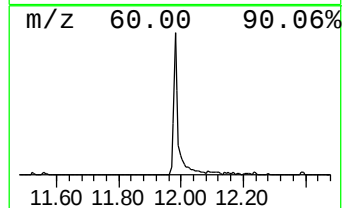
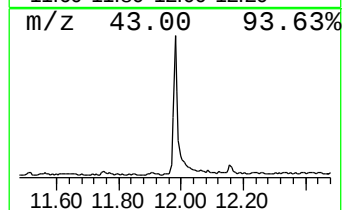
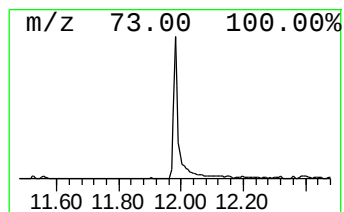
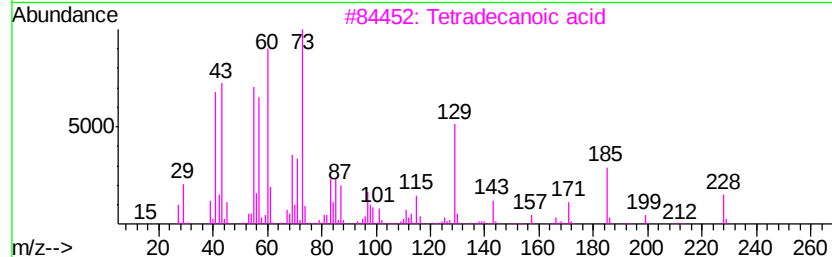
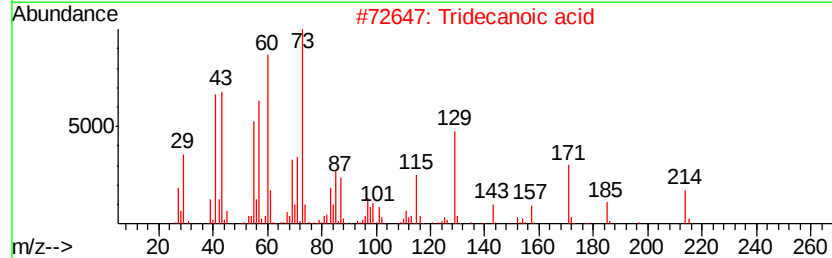
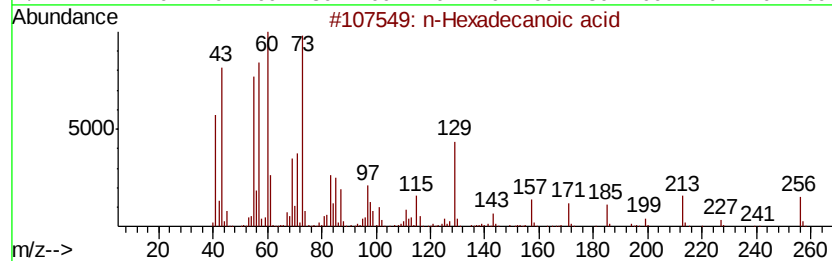
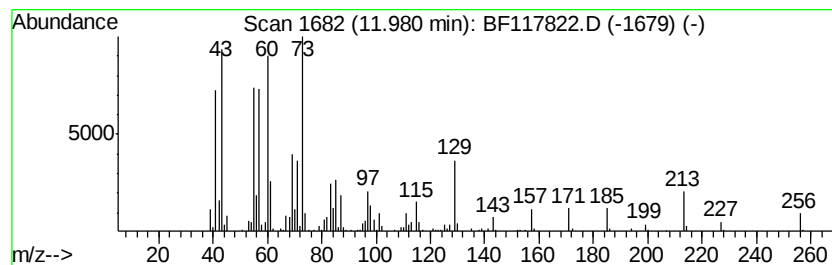
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.98	4.00 ng	418189	Phenanthrene-d10	11.46	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	95
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
5	Undecanoic acid	186	C11H22O2	000112-37-8	76



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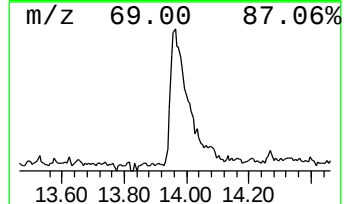
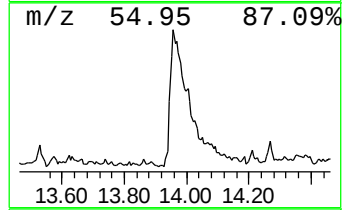
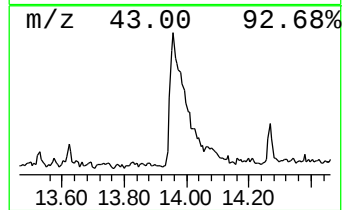
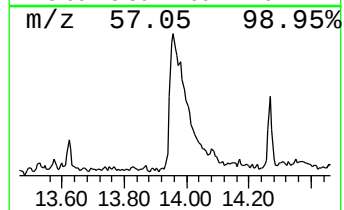
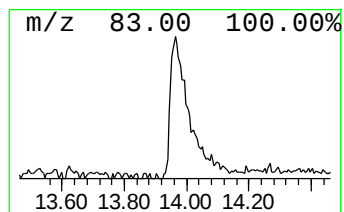
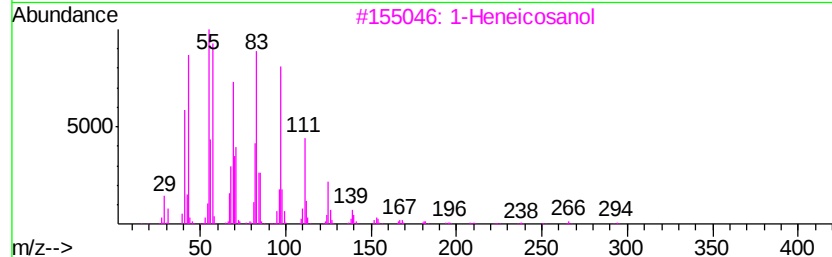
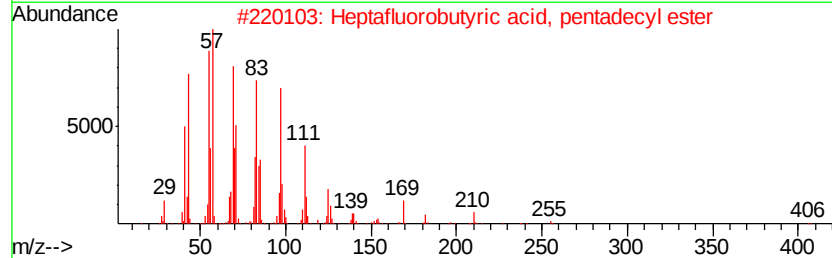
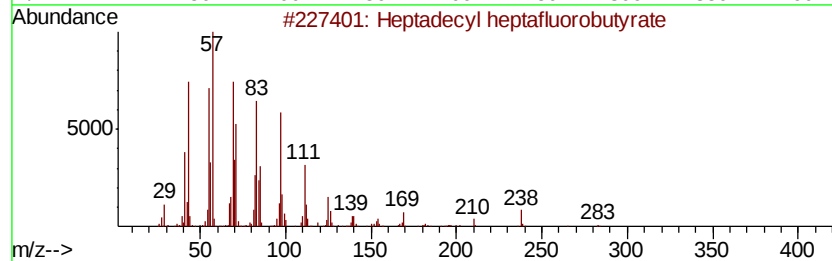
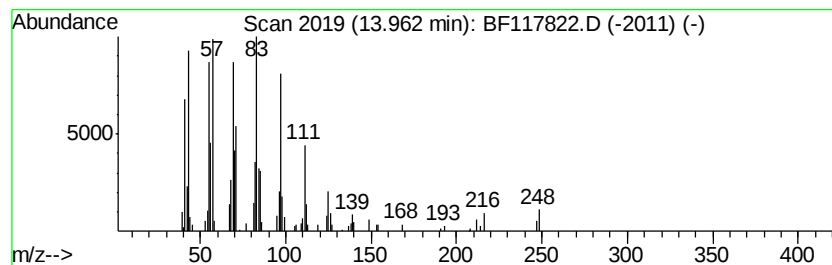
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.96	5.58 ng	532736	Chrysene-d12	14.10

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
3		1-Heneicosanol	312	C21H44O	015594-90-8	93
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	19.5	ng	1240830	1	6.92	1272770	20.0
2-Pentanone, 4-hy...	5.13	19.0	ng	1211050	1	6.92	1272770	20.0
unknown6.69	6.69	89.9	ng	5718950	1	6.92	1272770	20.0
n-Hexadecanoic acid	11.98	4.0	ng	418189	4	11.46	2090820	20.0
Heptadecyl heptaf...	13.96	5.6	ng	532736	5	14.10	1908460	20.0