

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF011419\
 Data File : BF112052.D
 Acq On : 14 Jan 2019 15:58
 Operator : JU/SJ
 Sample : K1129-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 P-1

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-BF010719.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	2.169	10	14	25	rVB	73961	119925	2.68%	0.312%
2	5.092	506	511	517	rBV	204320	250026	5.60%	0.651%
3	5.510	577	582	585	rBV	3874598	3635449	81.37%	9.461%
4	6.516	748	753	756	rBV	3999186	4261267	95.38%	11.090%
5	6.645	770	775	778	rBV	4533142	4217870	94.41%	10.977%
6	6.692	780	783	789	rVB	93240	82788	1.85%	0.215%
7	6.869	809	813	816	rBV	1248146	1065337	23.85%	2.772%
8	7.028	835	840	843	rBV	3305744	3037252	67.98%	7.904%
9	7.428	902	908	911	rBV	2370053	2314113	51.80%	6.022%
10	8.151	1026	1031	1034	rBV	1569395	1358334	30.40%	3.535%
11	9.227	1208	1214	1217	rBV	4630140	4467674	100.00%	11.627%
12	9.616	1276	1280	1283	rBV	1034591	804732	18.01%	2.094%
13	9.904	1325	1329	1333	rBV2	1980368	1771785	39.66%	4.611%
14	10.698	1459	1464	1467	rBV	3722624	3424244	76.64%	8.911%
15	11.392	1578	1582	1585	rBV	1442287	1194015	26.73%	3.107%
16	11.915	1668	1671	1679	rBV2	195871	182744	4.09%	0.476%
17	12.604	1785	1788	1793	rBV	75484	66272	1.48%	0.172%
18	12.833	1822	1827	1832	rBV	62249	80417	1.80%	0.209%
19	12.980	1847	1852	1855	rBV	3867939	3564312	79.78%	9.276%
20	13.862	1999	2002	2008	rBV2	177181	222903	4.99%	0.580%
21	14.033	2027	2031	2034	rBV	1144136	950426	21.27%	2.473%
22	14.192	2054	2058	2062	rBV	58782	59905	1.34%	0.156%
23	14.492	2106	2109	2114	rBV	69649	77036	1.72%	0.200%
24	14.798	2159	2161	2165	rVB	55427	54886	1.23%	0.143%
25	14.880	2171	2175	2178	rBV	43454	54207	1.21%	0.141%
26	15.145	2216	2220	2224	rBV	57827	81407	1.82%	0.212%
27	15.509	2277	2282	2291	rVB	777637	970737	21.73%	2.526%
28	15.962	2356	2359	2364	rVB	41508	56001	1.25%	0.146%

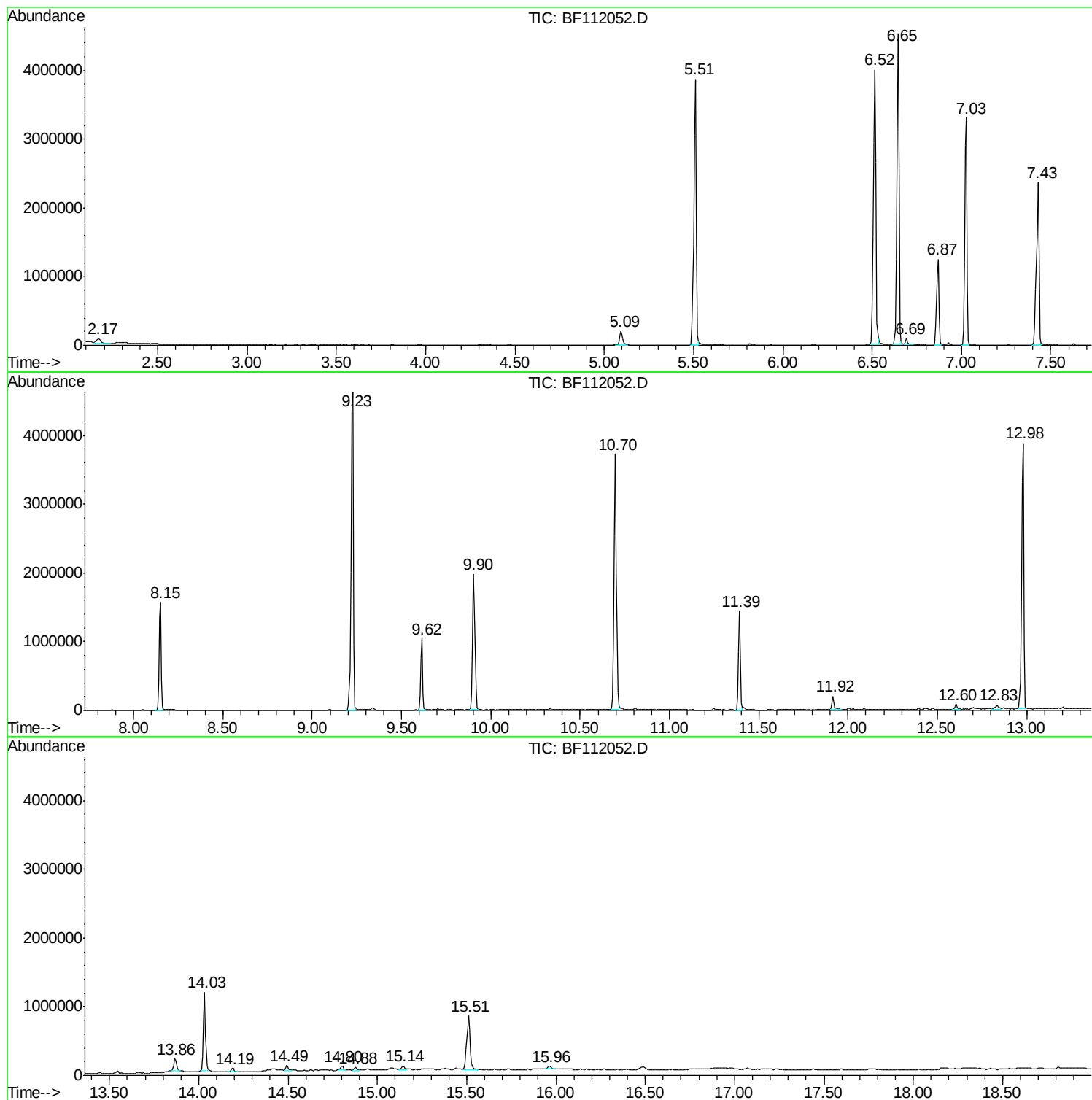
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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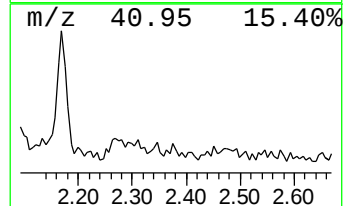
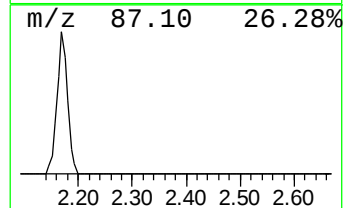
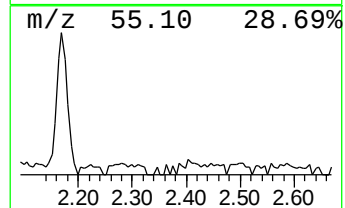
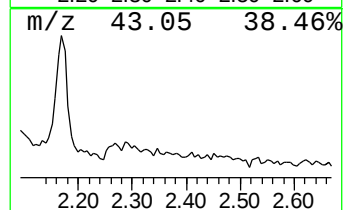
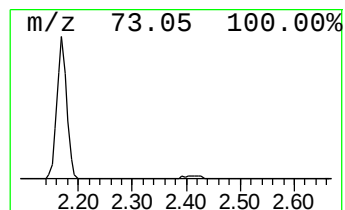
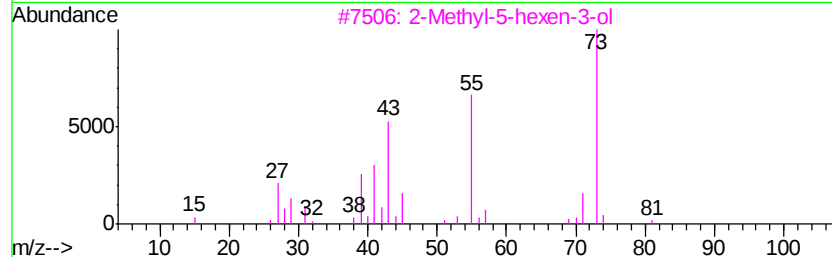
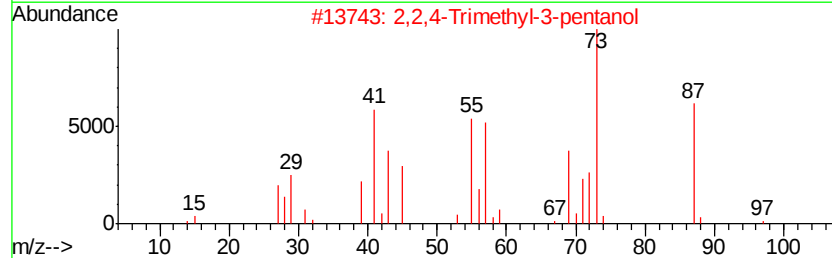
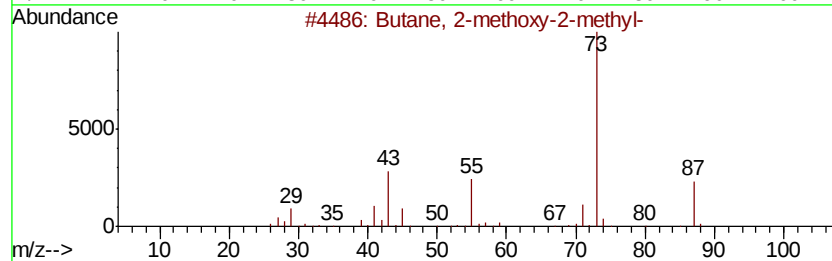
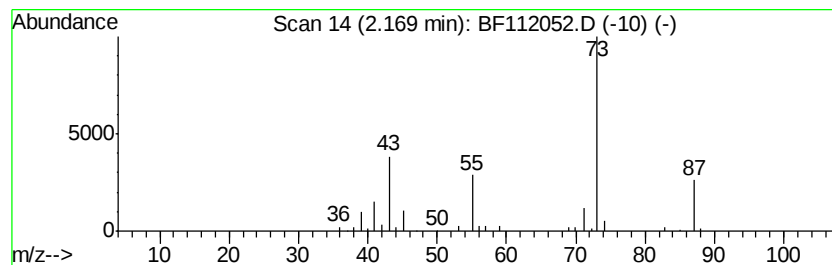
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF010719.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.25 ng	119925	1,4-Dichlorobenzene-d4	6.87

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	39
3		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
4		3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	25
5		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12



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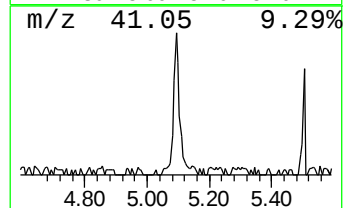
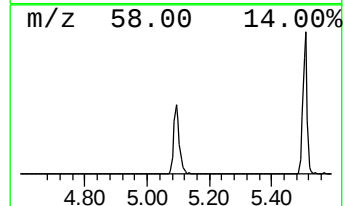
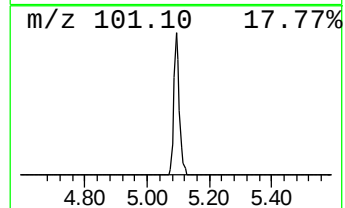
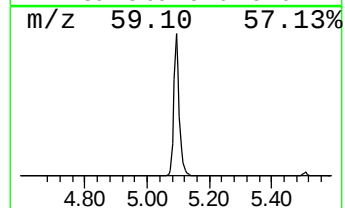
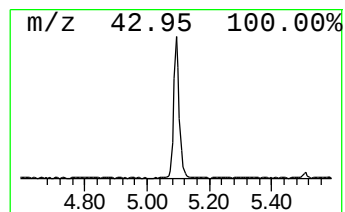
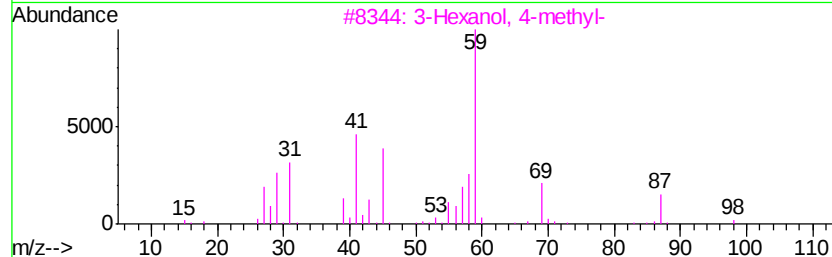
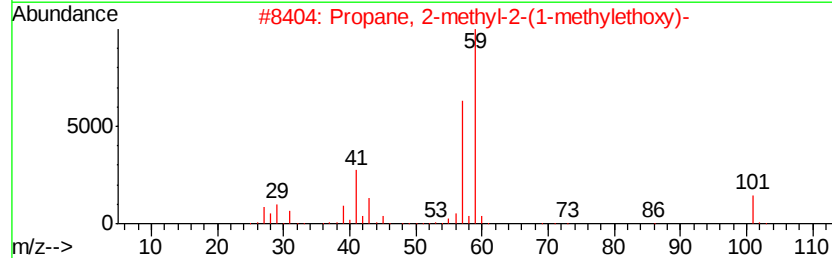
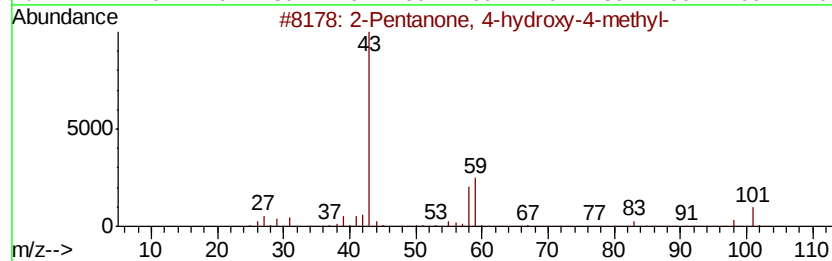
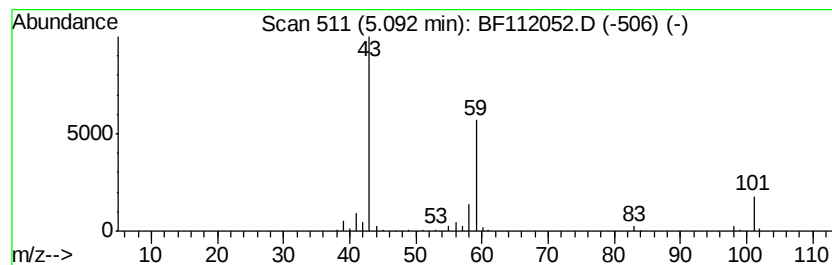
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.09	4.69 ng	250026	1,4-Dichlorobenzene-d4	6.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5			Silane, dimethyl-	60	C2H8Si	001111-74-6	9



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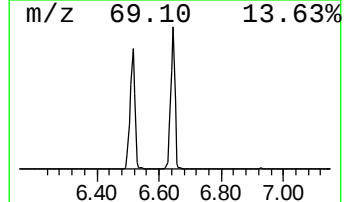
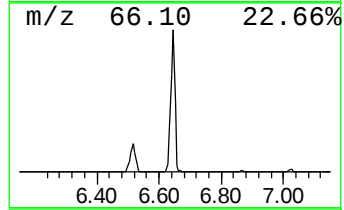
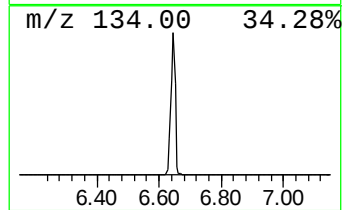
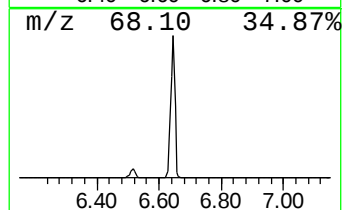
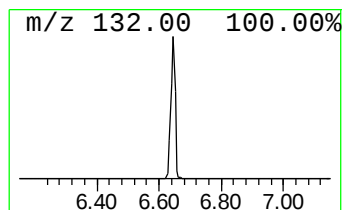
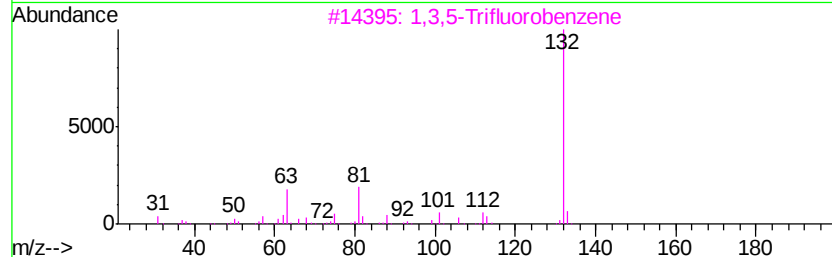
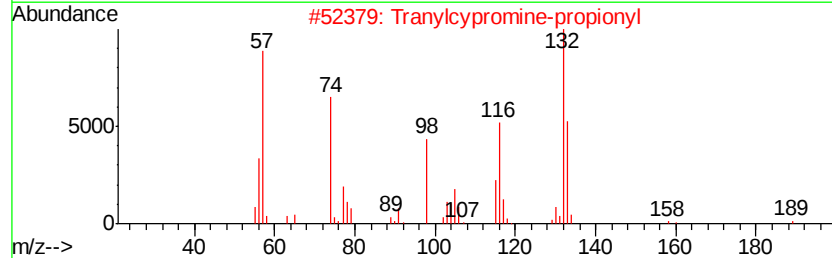
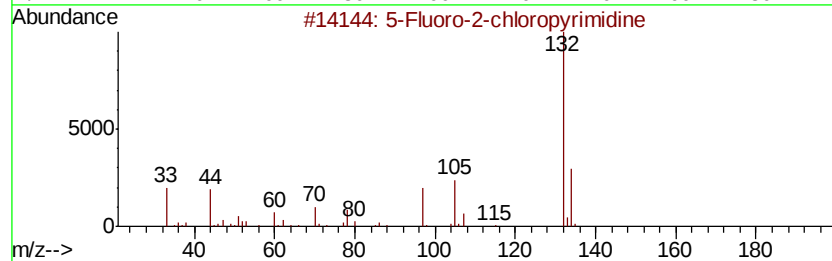
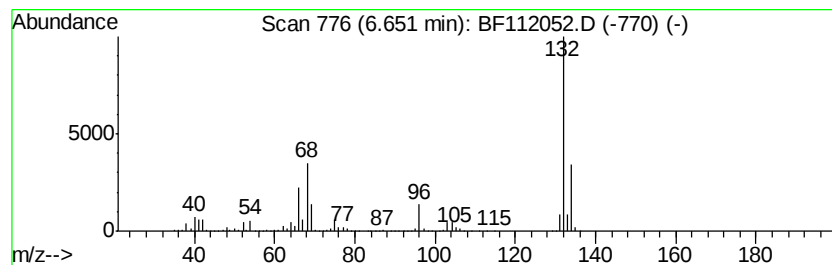
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Peak Number 3 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	79.18 ng	4217870	1,4-Dichlorobenzene-d4	6.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
2		Tranlycypromine-propionyl	189	C12H15NO	1000123-86-3	12
3		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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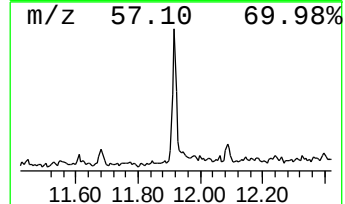
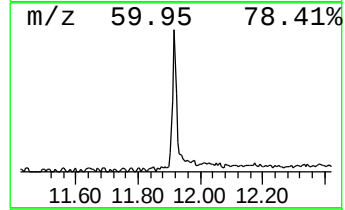
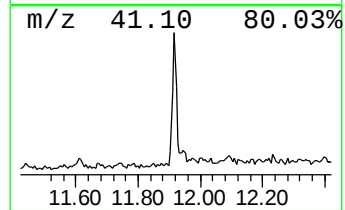
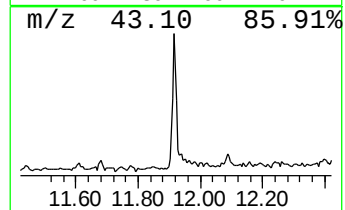
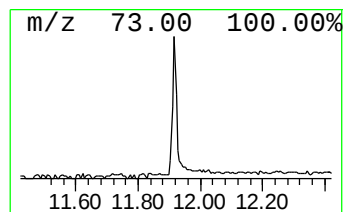
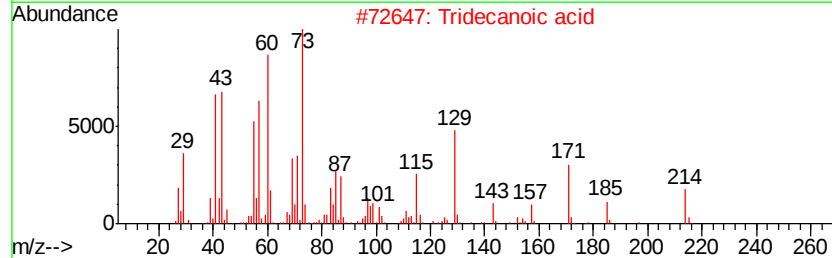
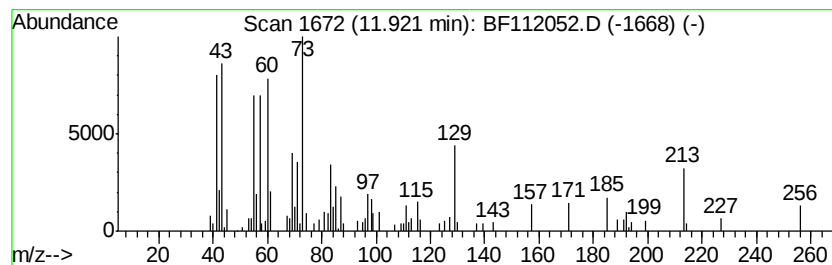
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.92	3.06 ng	182744	Phenanthrene-d10	11.39

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	68



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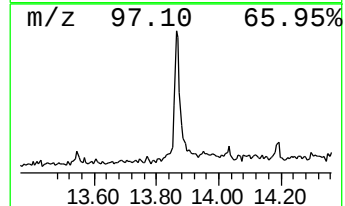
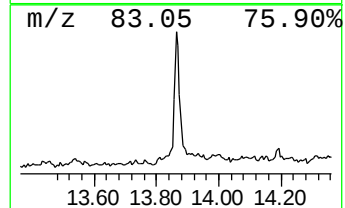
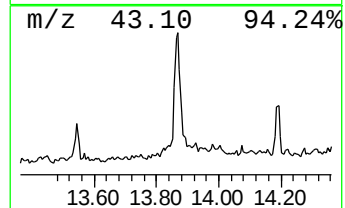
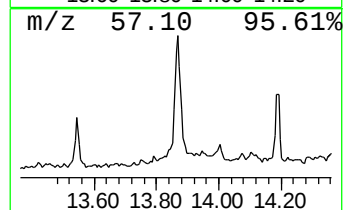
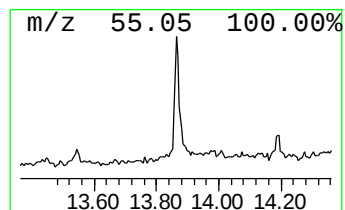
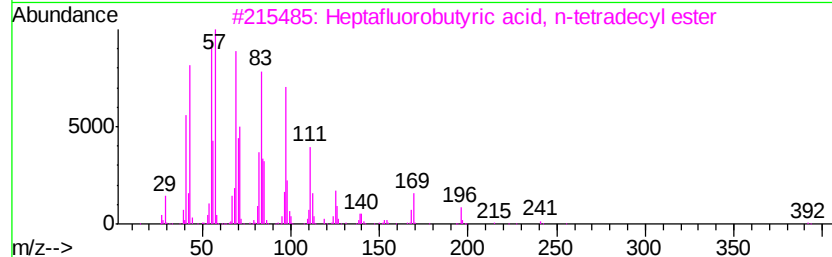
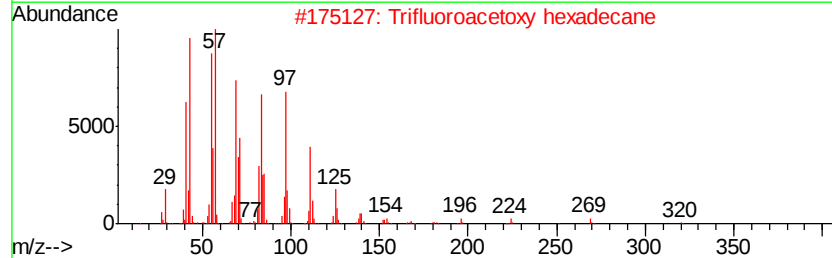
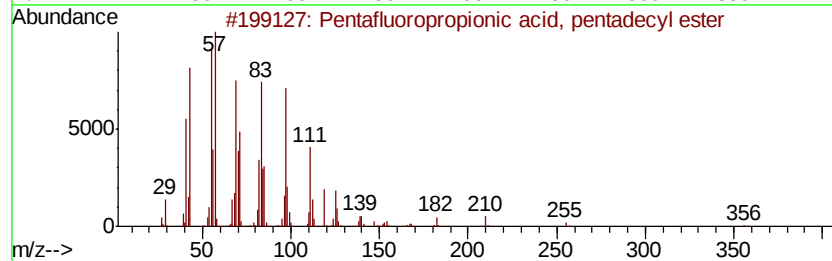
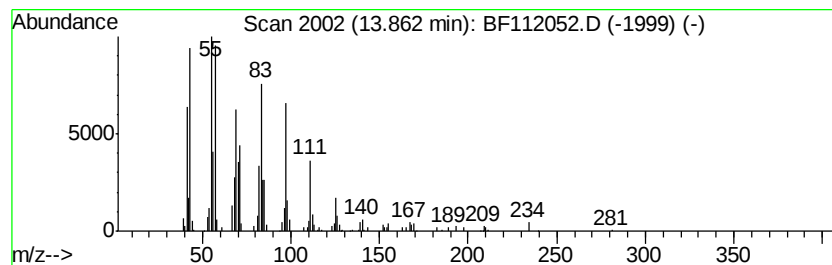
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.86	4.69 ng	222903	Chrysene-d12	14.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
5		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.17	2.3	ng	119925	1	6.87	1065340	20.0
2-Pentanone, 4-hy...	5.09	4.7	ng	250026	1	6.87	1065340	20.0
unknown6.65	6.65	79.2	ng	4217870	1	6.87	1065340	20.0
n-Hexadecanoic acid	11.92	3.1	ng	182744	4	11.39	1194020	20.0
Pentafluoropropio...	13.86	4.7	ng	222903	5	14.03	950426	20.0