

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
 Data File : BF095696.D
 Acq On : 6 Jun 2017 3:30
 Operator : SJ/MA
 Sample : I3444-03 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 BU-RO-240-060117

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-BF060517.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	1.602	9	11	38	rBV	492513	950912	88.37%	8.891%
2	4.590	516	519	540	rBV	29684	71703	6.66%	0.670%
3	5.295	635	639	675	rBV	341272	773391	71.87%	7.231%
4	6.954	918	921	934	rBV	444500	851200	79.10%	7.959%
5	7.054	934	938	958	rVB	682763	1076076	100.00%	10.061%
6	7.401	993	997	1014	rBB	345681	464910	43.20%	4.347%
7	7.636	1032	1037	1050	rBV	487431	621483	57.75%	5.811%
8	8.307	1148	1151	1173	rBV	276642	423134	39.32%	3.956%
9	9.430	1337	1342	1355	rBV	469100	590674	54.89%	5.523%
10	11.207	1639	1644	1656	rVB	773784	878655	81.65%	8.215%
11	11.901	1757	1762	1769	rBV	69399	80125	7.45%	0.749%
12	12.254	1816	1822	1827	rBV2	448558	567675	52.75%	5.308%
13	12.301	1827	1830	1835	rVB3	18730	23143	2.15%	0.216%
14	13.113	1963	1968	1972	rVB	18992	21137	1.96%	0.198%
15	13.542	2037	2041	2050	rBV	264992	344105	31.98%	3.217%
16	13.883	2094	2099	2107	rBV2	20794	40032	3.72%	0.374%
17	14.612	2218	2223	2224	rBV	15996	17317	1.61%	0.162%
18	14.642	2224	2228	2233	rVV	380365	482473	44.84%	4.511%
19	14.683	2233	2235	2242	rVB	35939	43842	4.07%	0.410%
20	15.289	2334	2338	2344	rBV2	13702	20671	1.92%	0.193%
21	15.442	2359	2364	2369	rBV3	22757	33725	3.13%	0.315%
22	15.495	2369	2373	2378	rVB2	12260	15407	1.43%	0.144%
23	15.601	2388	2391	2395	rBV2	15656	17916	1.66%	0.168%
24	15.654	2395	2400	2410	rVB3	33963	48382	4.50%	0.452%
25	15.901	2438	2442	2446	rBV4	14436	20259	1.88%	0.189%
26	16.259	2499	2503	2507	rBV2	12772	15637	1.45%	0.146%
27	16.412	2526	2529	2532	rVV2	67613	70062	6.51%	0.655%
28	16.453	2532	2536	2543	rVB	99706	163768	15.22%	1.531%
29	16.577	2552	2557	2560	rBV6	9998	17891	1.66%	0.167%
30	16.759	2584	2588	2593	rBV	102884	125726	11.68%	1.176%
31	16.953	2618	2621	2624	rBV4	16862	18647	1.73%	0.174%
32	17.012	2626	2631	2636	rVB	610759	665414	61.84%	6.221%
33	17.089	2641	2644	2647	rBV5	10674	14861	1.38%	0.139%
34	17.236	2660	2669	2673	rVB4	23467	45890	4.26%	0.429%

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Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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35	17.318	2680	2683	2688	rVB	17438	18350	1.71%	0.172%
36	17.371	2688	2692	2693	rBV2	17039	19488	1.81%	0.182%
37	17.512	2714	2716	2720	rBV4	10463	15103	1.40%	0.141%
38	17.577	2724	2727	2730	rVV4	15796	17867	1.66%	0.167%
39	17.712	2747	2750	2751	rBV3	16530	17207	1.60%	0.161%
40	17.812	2765	2767	2770	rBV4	12184	12494	1.16%	0.117%
41	18.271	2842	2845	2853	rVB10	31820	73474	6.83%	0.687%
42	18.353	2855	2859	2863	rBV	448587	527895	49.06%	4.936%
43	20.024	3139	3143	3149	rBV	296677	377311	35.06%	3.528%

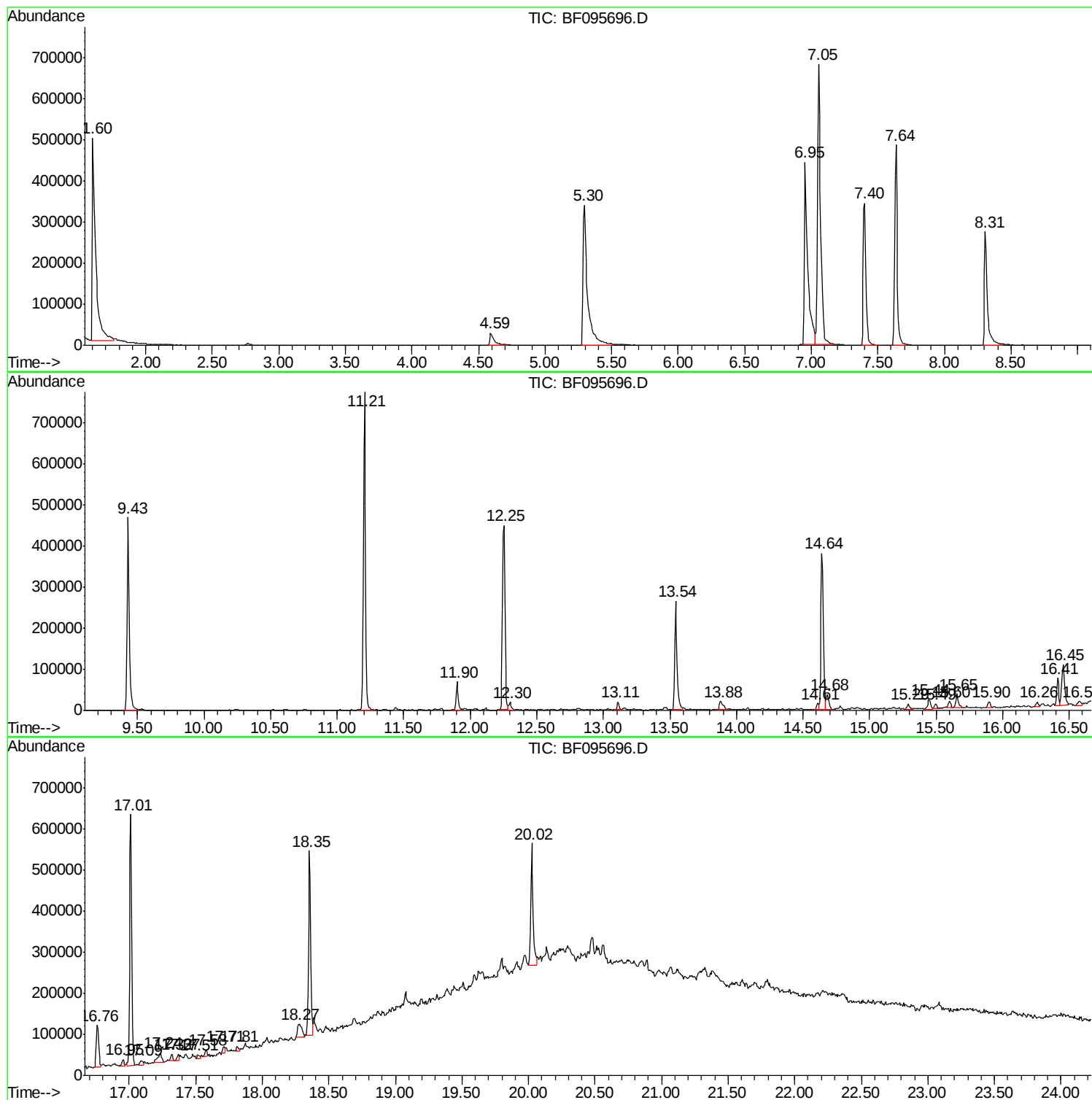
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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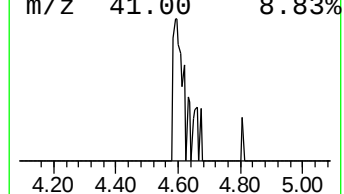
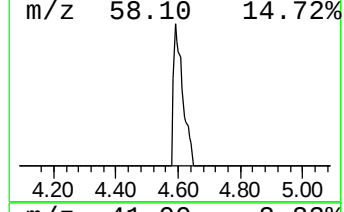
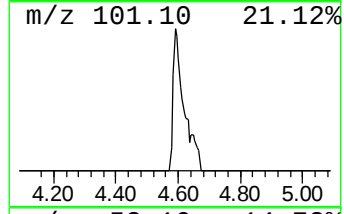
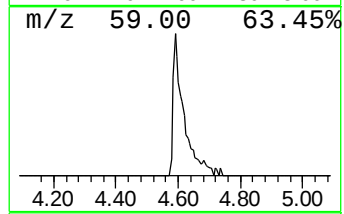
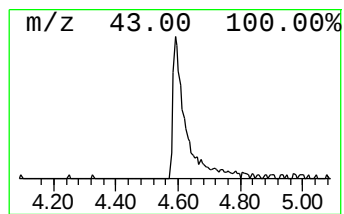
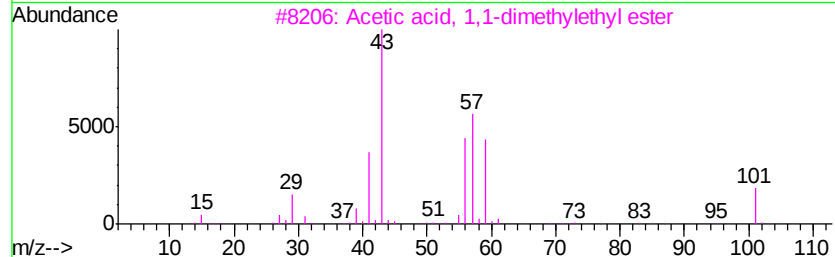
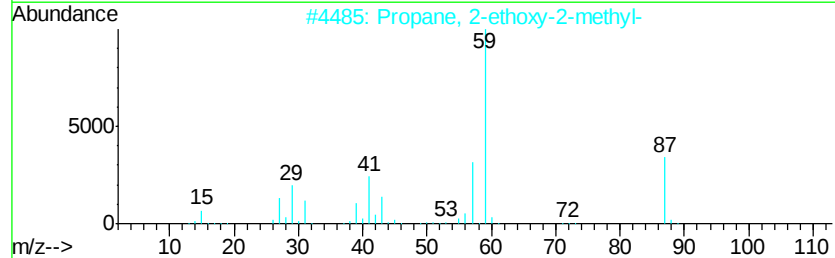
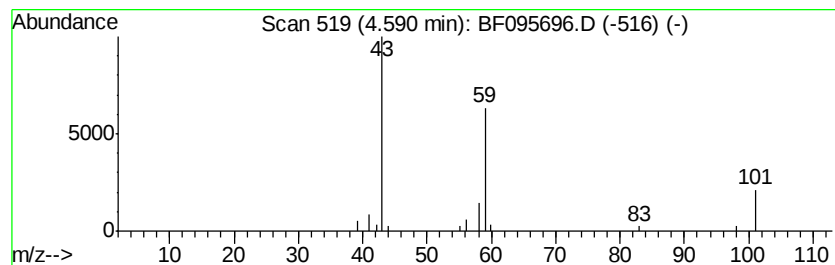
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.59	3.08 ng	71703	1,4-Dichlorobenzene-d4	7.40

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9
4			1,2-Butanediol	90	C4H10O2	000584-03-2	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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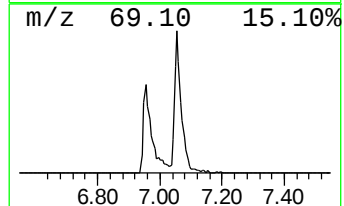
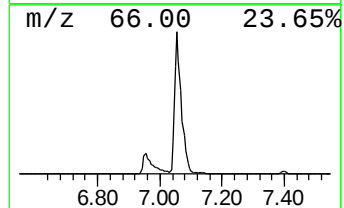
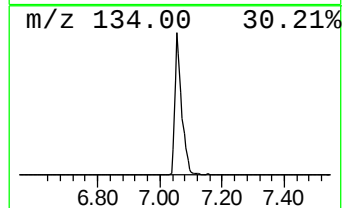
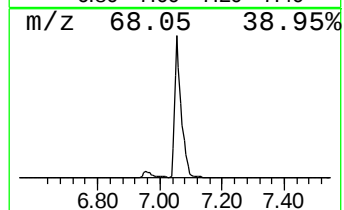
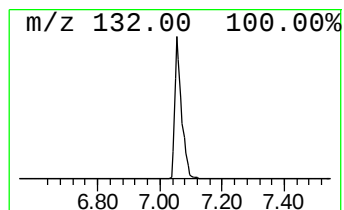
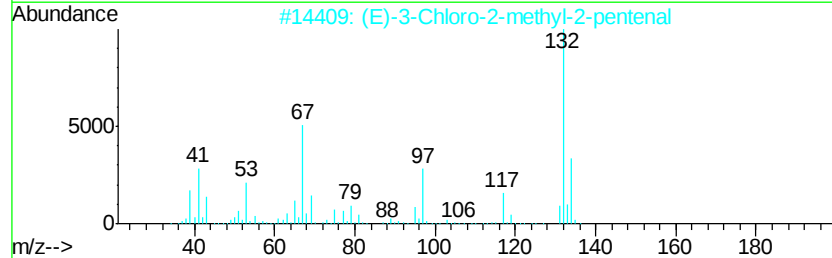
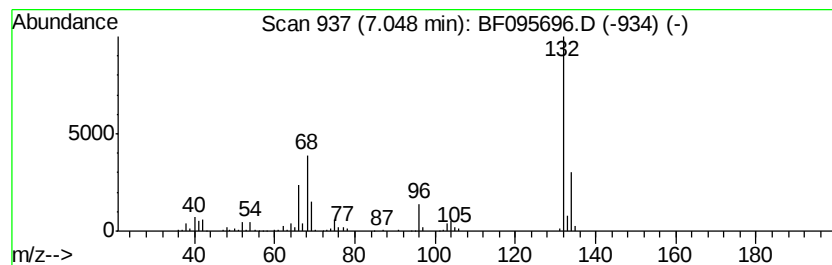
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown7.05 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.05	46.29 ng	1076080	1,4-Dichlorobenzene-d4	7.40

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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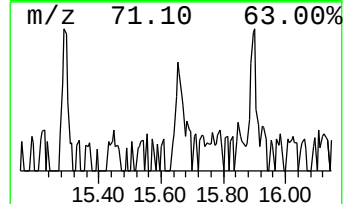
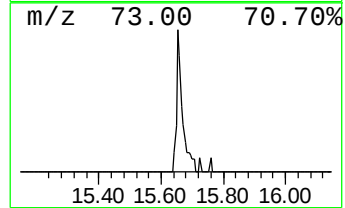
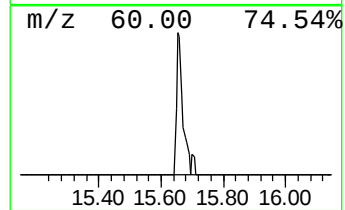
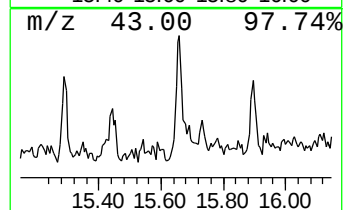
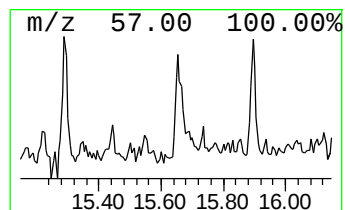
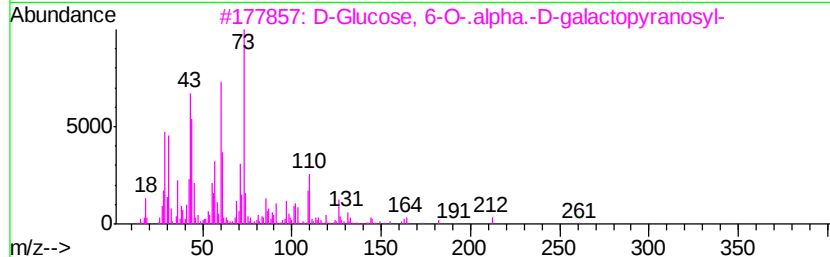
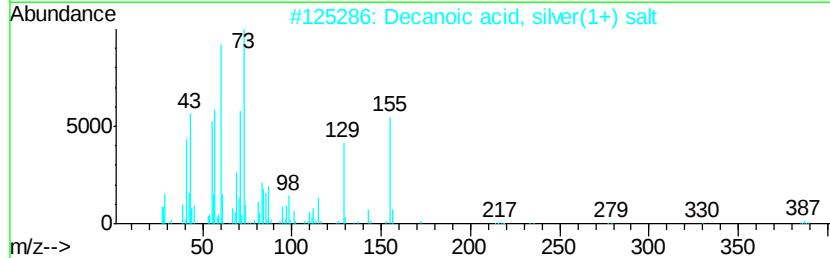
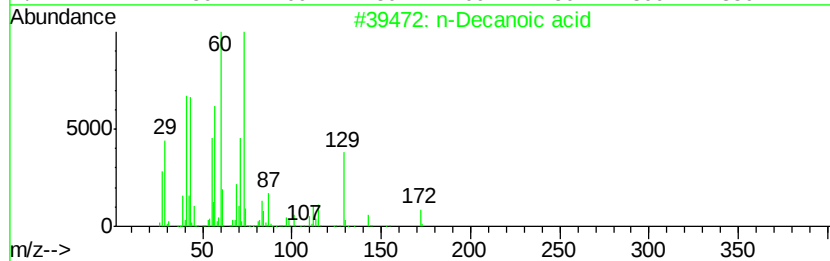
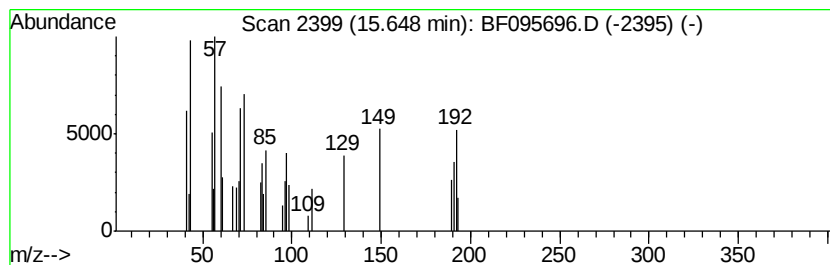
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Peak Number 5 unknown15.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.65	2.01 ng	48382	Phenanthrene-d10	14.64

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Decanoic acid	172	C10H20O2	000334-48-5	47
2		Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47
3		D-Glucose, 6-O-.alpha.-D-galacto...	342	C12H22O11	000585-99-9	43
4		Lactose	342	C12H22O11	000063-42-3	38
5		Dodecanoic acid	200	C12H24O2	000143-07-7	38



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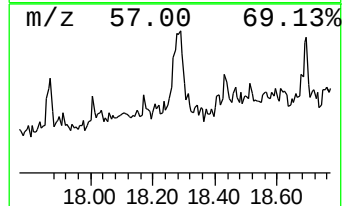
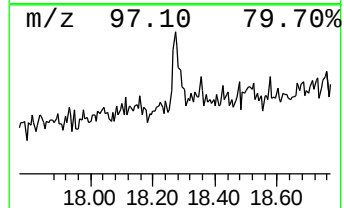
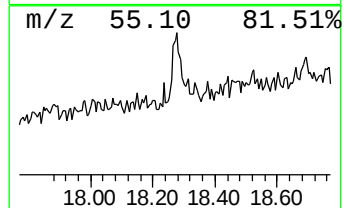
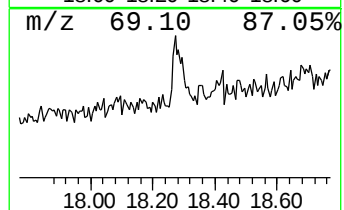
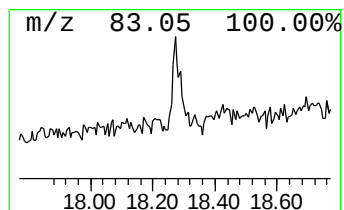
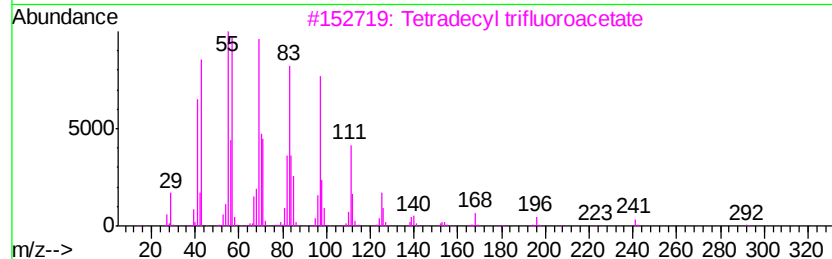
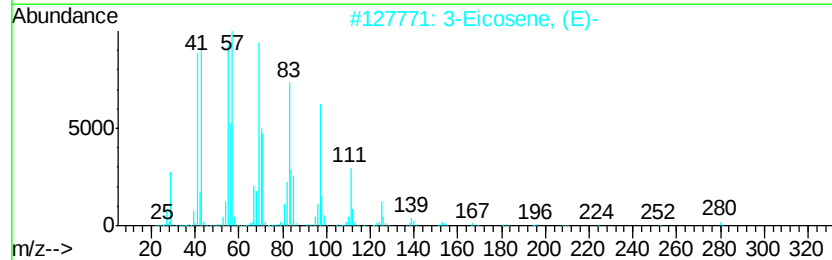
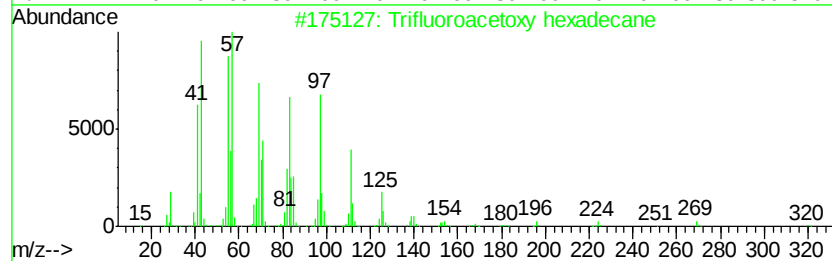
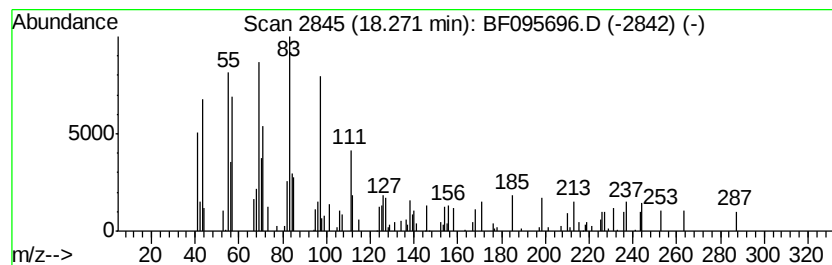
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.27	2.78 ng	73474	Chrysene-d12	18.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	62
2		3-Eicosene, (E)-	280	C20H40	074685-33-9	62
3		Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	62
4		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	53
5		1-Pentadecene	210	C15H30	013360-61-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.59	3.1	ng	71703	1	7.40	464910	20.0
unknown7.05	7.05	46.3	ng	1076080	1	7.40	464910	20.0
unknown15.65	15.65	2.0	ng	48382	4	14.64	482473	20.0
Trifluoroacetoxy ...	18.27	2.8	ng	73474	5	18.35	527895	20.0