

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011224\
 Data File : BF137052.D
 Acq On : 12 Jan 2024 16:57
 Operator : CG\JU
 Sample : P1118-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WC-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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137052.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	8	11	19	rVB	9213	14419	1.40%	0.186%
2	5.016	494	498	509	rVB	56785	66704	6.49%	0.862%
3	5.428	565	568	583	rBV	914194	854442	83.18%	11.039%
4	6.434	735	739	757	rBV	1011632	886855	86.33%	11.458%
5	6.781	795	798	802	rBV	414179	342486	33.34%	4.425%
6	7.345	890	894	897	rBV	670077	535218	52.10%	6.915%
7	8.057	1012	1015	1019	rBV	515754	429263	41.79%	5.546%
8	8.386	1066	1071	1082	rBV3	7898	18627	1.81%	0.241%
9	9.133	1194	1198	1209	rBV	1182481	1027252	100.00%	13.272%
10	9.816	1310	1314	1323	rBV	579384	473865	46.13%	6.122%
11	9.916	1327	1331	1336	rVB2	10799	14346	1.40%	0.185%
12	10.610	1446	1449	1459	rBV	639500	564895	54.99%	7.298%
13	11.310	1564	1568	1571	rBV	512196	430768	41.93%	5.565%
14	11.333	1571	1572	1579	rVB	27897	17310	1.69%	0.224%
15	11.839	1655	1658	1670	rBV2	132670	141814	13.81%	1.832%
16	12.533	1772	1776	1779	rBV	47720	43002	4.19%	0.556%
17	12.633	1789	1793	1799	rBV	26941	37191	3.62%	0.481%
18	12.763	1809	1815	1819	rVB	38016	39613	3.86%	0.512%
19	12.904	1835	1839	1842	rBV	865561	721023	70.19%	9.316%
20	13.886	2000	2006	2012	rBV9	17658	52436	5.10%	0.677%
21	13.968	2016	2020	2023	rVV	354536	348112	33.89%	4.498%
22	13.992	2023	2024	2030	rVB	27624	23525	2.29%	0.304%
23	14.433	2096	2099	2102	rBV3	14256	13414	1.31%	0.173%
24	14.645	2133	2135	2139	rBV3	11908	14880	1.45%	0.192%
25	14.727	2146	2149	2156	rVB2	20996	31806	3.10%	0.411%
26	14.815	2161	2164	2168	rVB2	19247	19044	1.85%	0.246%
27	15.021	2195	2199	2202	rBV	25094	38433	3.74%	0.497%
28	15.086	2207	2210	2215	rVB2	11868	14762	1.44%	0.191%
29	15.227	2230	2234	2239	rBV7	6674	13306	1.30%	0.172%
30	15.327	2249	2251	2254	rBV	14177	15203	1.48%	0.196%
31	15.392	2259	2262	2268	rVB	23035	29169	2.84%	0.377%
32	15.457	2268	2273	2285	rBV	300610	400064	38.95%	5.169%
33	15.921	2348	2352	2355	rBV4	12359	15691	1.53%	0.203%
34	16.986	2528	2533	2540	rVB3	13261	29198	2.84%	0.377%
35	17.062	2540	2546	2552	rVB3	9890	21885	2.13%	0.283%

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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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

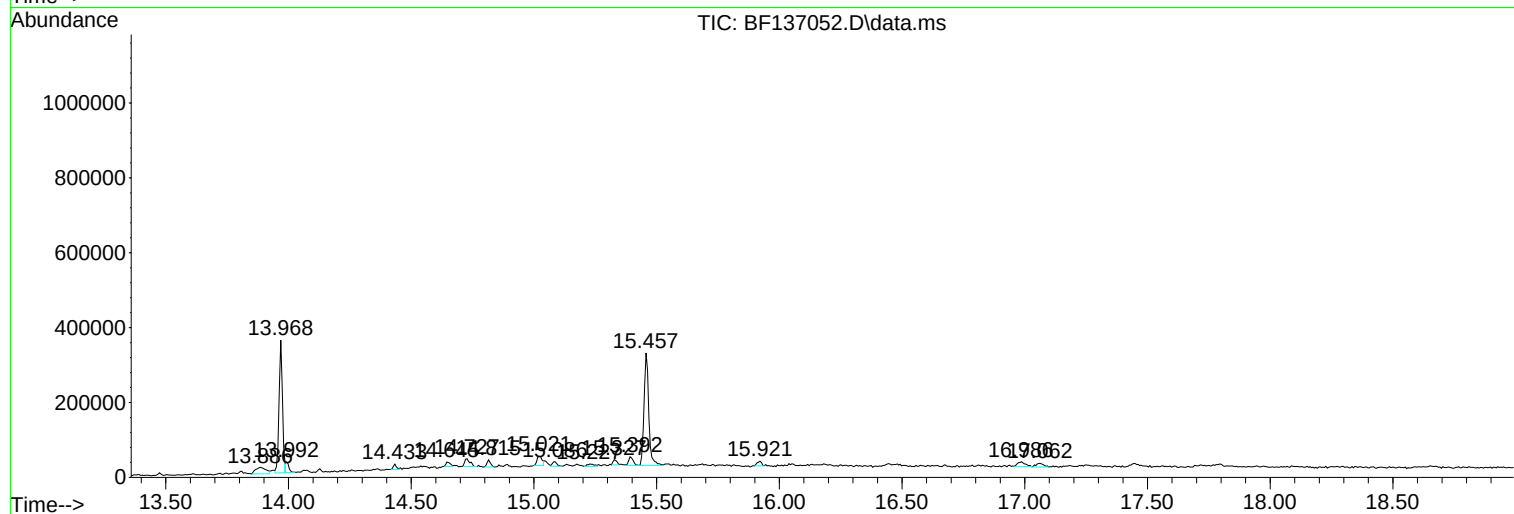
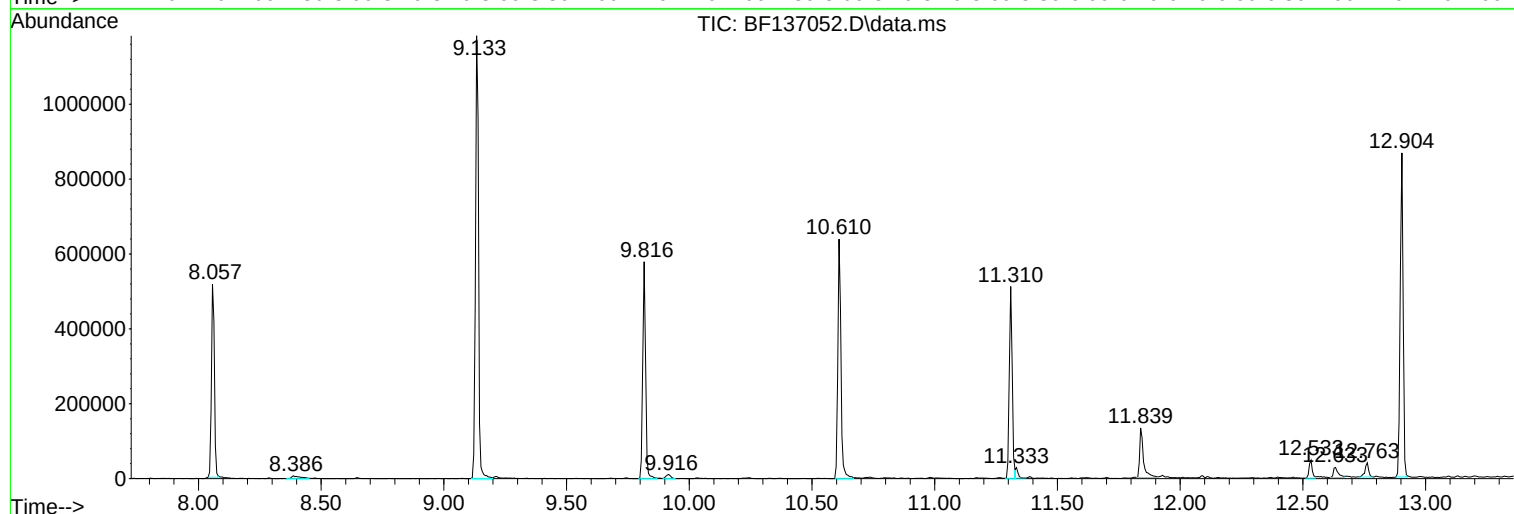
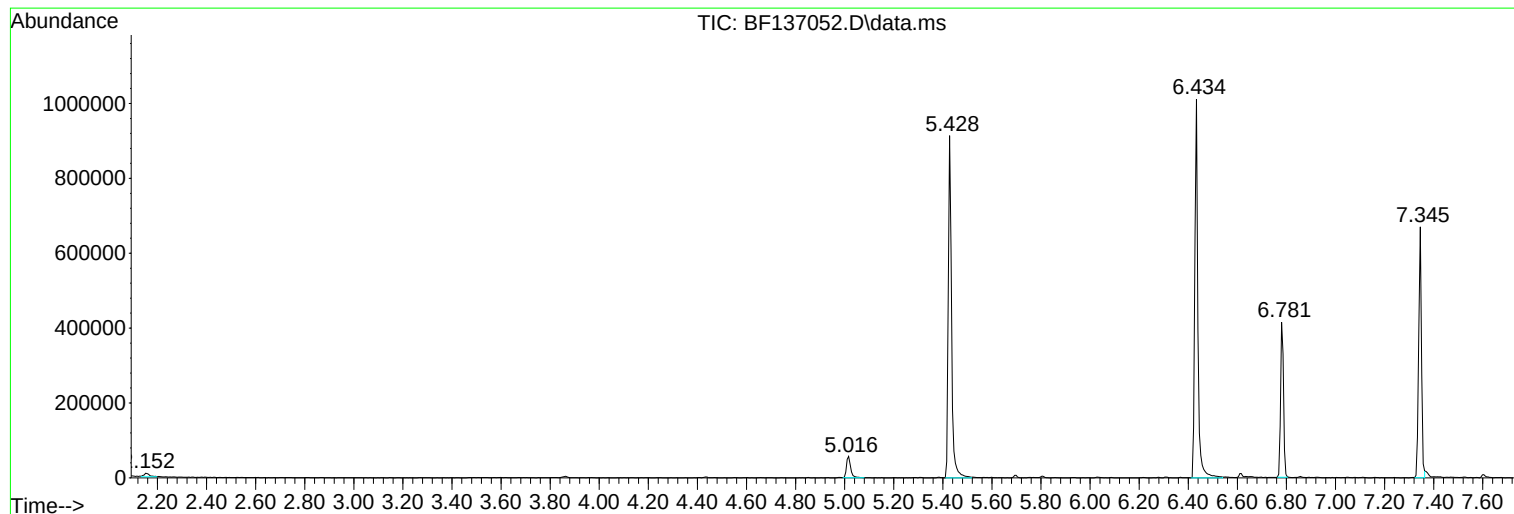
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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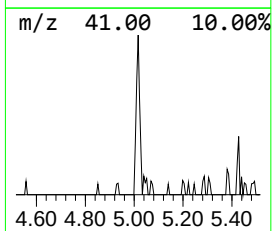
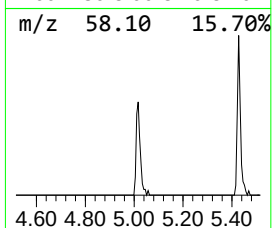
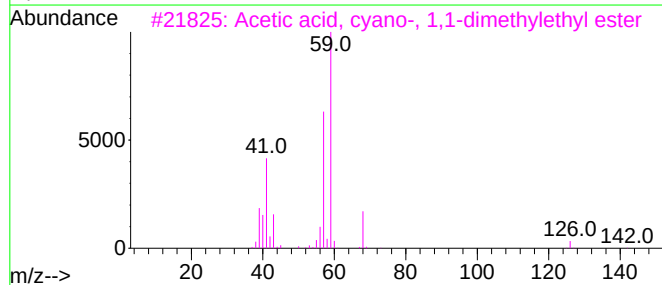
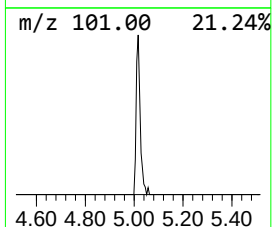
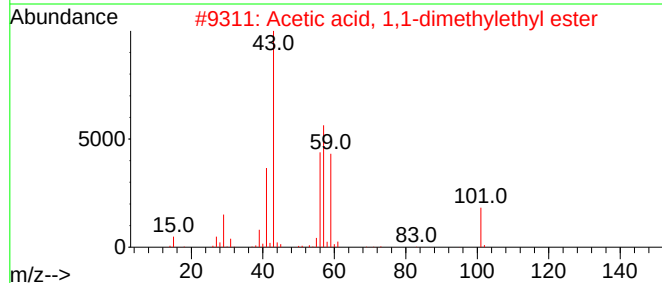
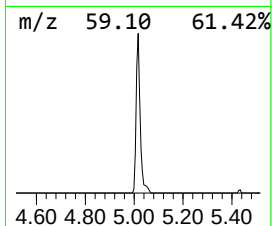
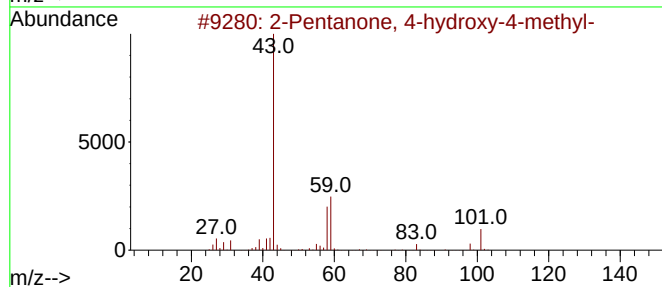
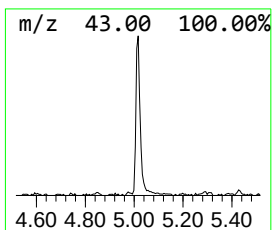
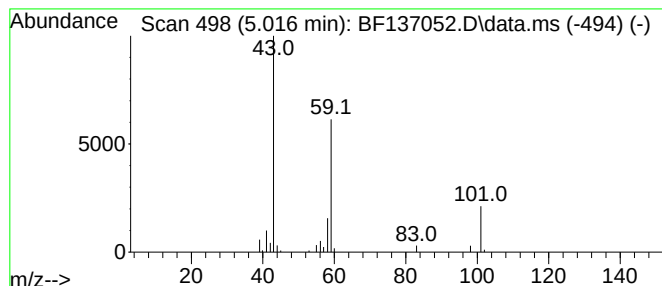
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.90 ng	66704	1,4-Dichlorobenzene-d4	6.781

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		



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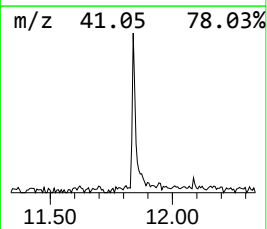
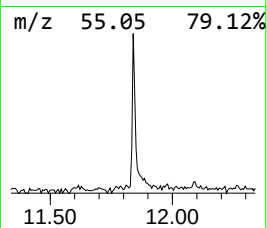
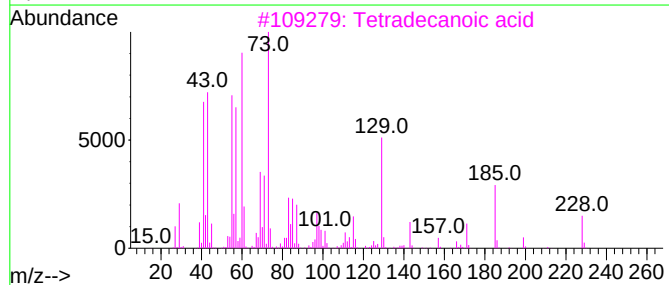
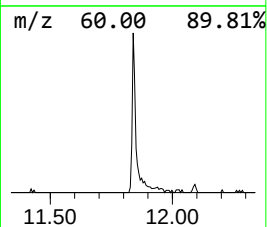
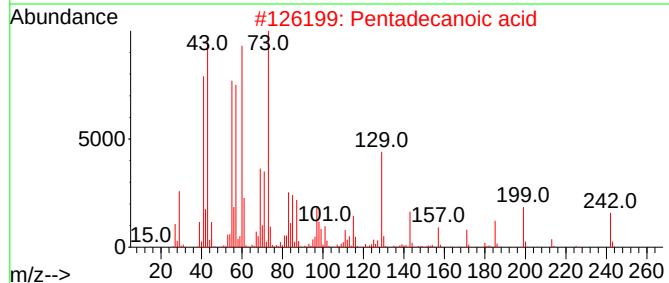
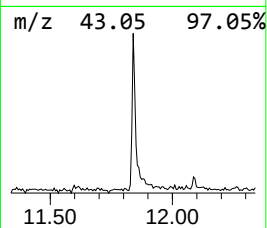
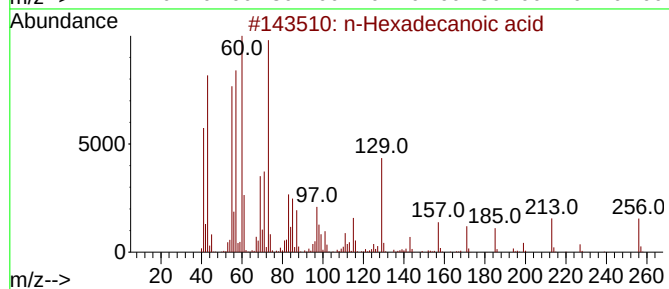
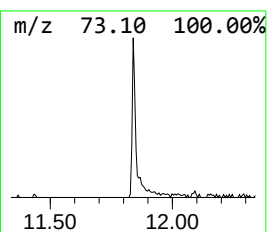
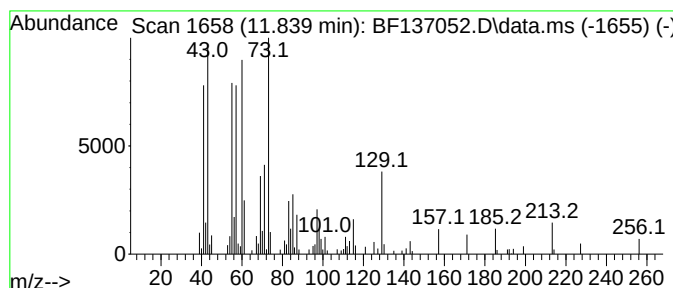
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.839	6.58 ng	141814	Phenanthrene-d10	11.310	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Tridecanoic acid	214	C13H26O2	000638-53-9	80
5	Octanoic acid	144	C8H16O2	000124-07-2	43



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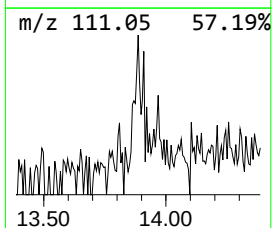
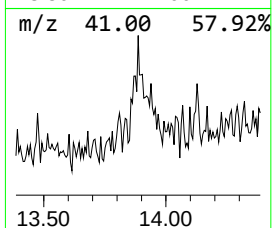
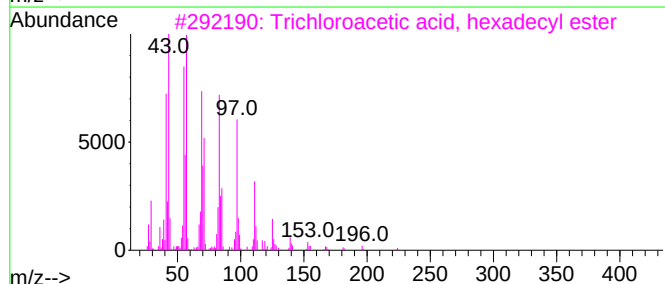
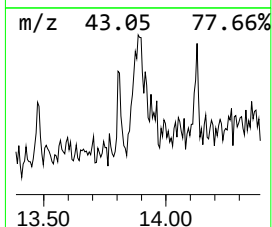
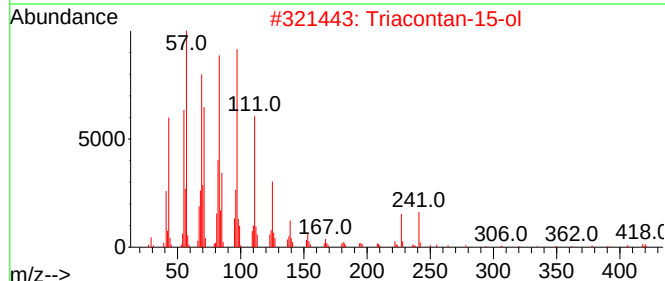
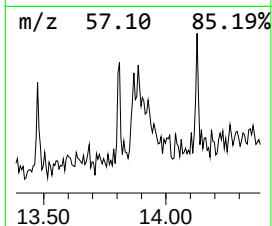
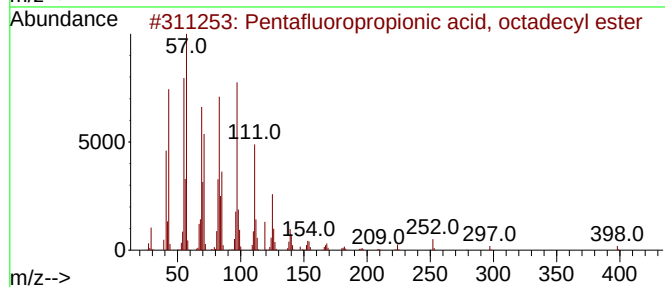
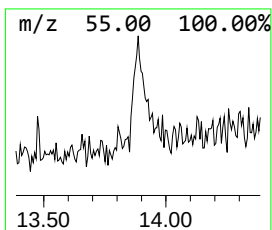
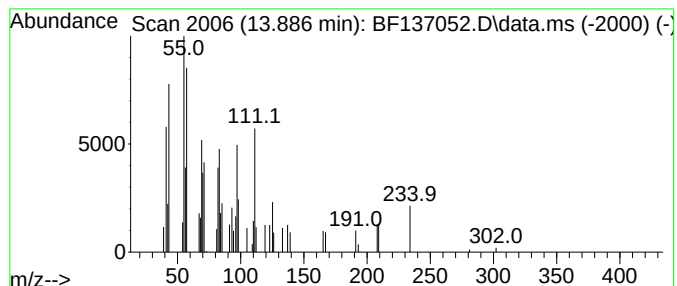
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.01 ng	52436	Chrysene-d12	13.969

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	62
2			Triacontan-15-ol	438	C30H62O	031849-26-0	58
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	58
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	53
5			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	53



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	3.9	ng	66704	1	6.781	342486	20.0
n-Hexadecanoic ...	11.839	6.6	ng	141814	4	11.310	430768	20.0
Pentafluoroprop...	13.886	3.0	ng	52436	5	13.969	348112	20.0