

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
 Data File : BF125451.D
 Acq On : 13 Sep 2021 19:08
 Operator : JU/CG
 Sample : M3684-20
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A006015

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-BF081821.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125451.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.193	10	18	29	rVB	1605932	2103879	54.08%	6.927%
2	2.299	32	36	46	rVB	56050	74134	1.91%	0.244%
3	5.110	510	514	526	rVB	208513	260986	6.71%	0.859%
4	5.516	578	583	586	rBV	3198736	3374692	86.74%	11.111%
5	6.522	749	754	757	rBV	3275369	3349861	86.10%	11.029%
6	6.881	812	815	819	rBV	1087442	987012	25.37%	3.250%
7	7.451	906	912	915	rBV	2241089	2216392	56.97%	7.297%
8	8.075	1014	1018	1030	rBV2	84426	249970	6.42%	0.823%
9	8.169	1030	1034	1049	rVB	1535908	1369723	35.21%	4.510%
10	9.245	1212	1217	1220	rBV	4503974	3890642	100.00%	12.810%
11	9.928	1329	1333	1336	rBV	1778928	1475000	37.91%	4.856%
12	10.716	1463	1467	1481	rVB	2627606	2597701	66.77%	8.553%
13	11.416	1582	1586	1589	rBV	1840844	1554828	39.96%	5.119%
14	11.439	1589	1590	1594	rVB	130955	73245	1.88%	0.241%
15	11.933	1669	1674	1679	rBV2	165102	188989	4.86%	0.622%
16	12.633	1789	1793	1800	rBV	155496	139736	3.59%	0.460%
17	12.721	1805	1808	1813	rBV3	47744	53123	1.37%	0.175%
18	12.863	1826	1832	1835	rBV	137047	141845	3.65%	0.467%
19	13.004	1852	1856	1859	rBV	4356683	3879260	99.71%	12.772%
20	13.951	2010	2017	2029	rBV5	83938	306726	7.88%	1.010%
21	14.063	2032	2036	2039	rBV	1201645	1048384	26.95%	3.452%
22	15.121	2212	2216	2219	rBV	42855	63641	1.64%	0.210%
23	15.557	2285	2290	2307	rVB	713712	972861	25.01%	3.203%

Sum of corrected areas: 30372630

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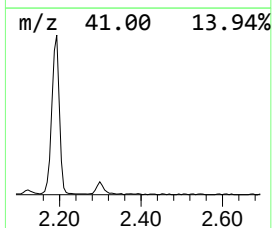
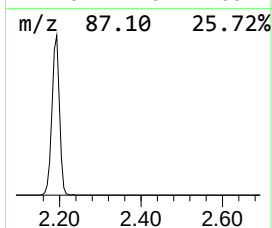
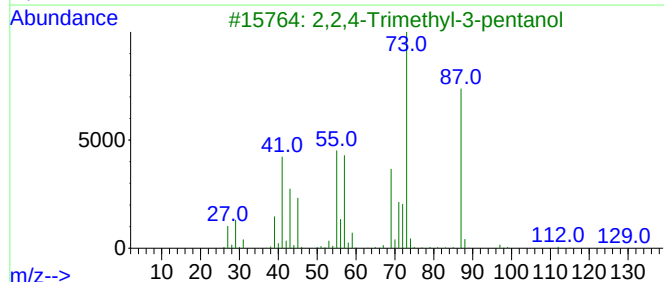
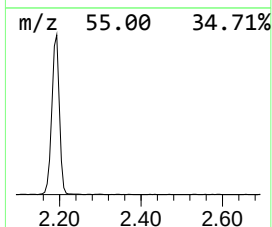
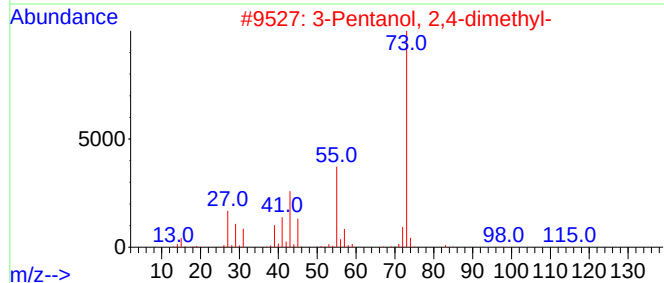
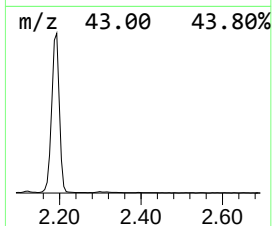
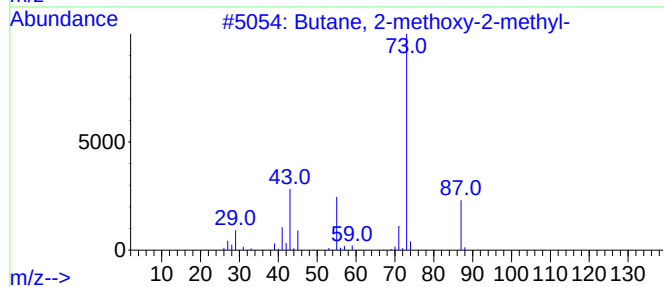
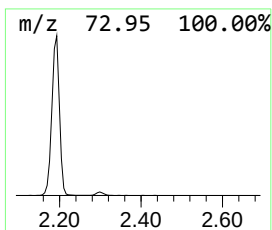
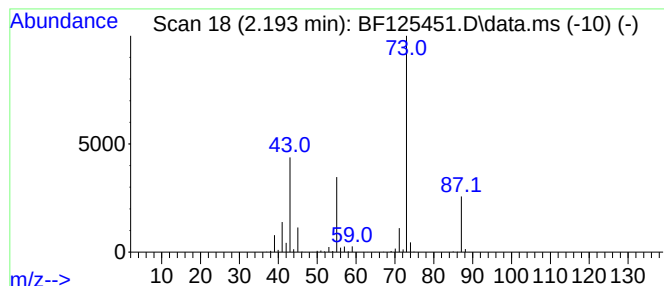
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.193	42.63 ng	2103880	1,4-Dichlorobenzene-d4	6.887

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17



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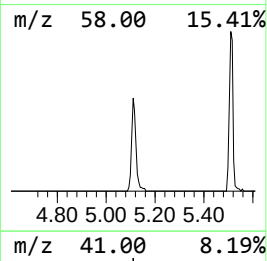
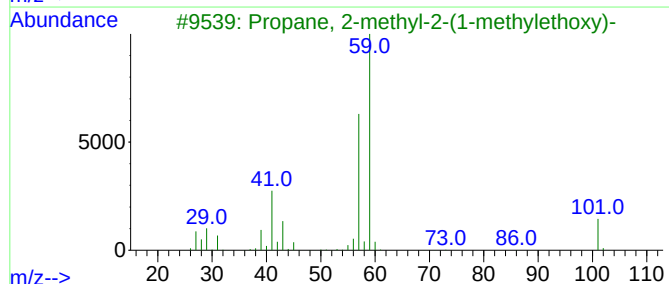
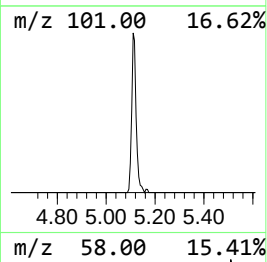
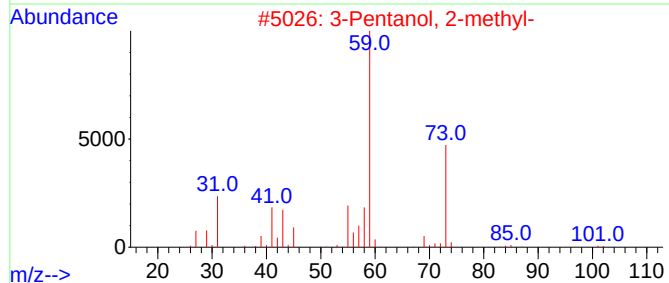
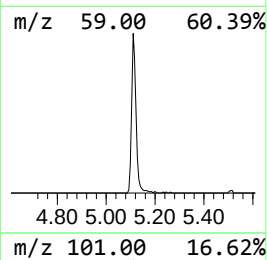
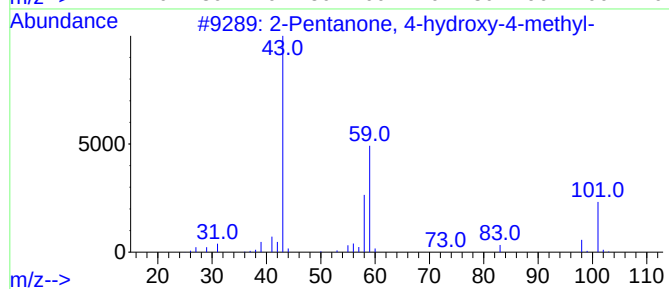
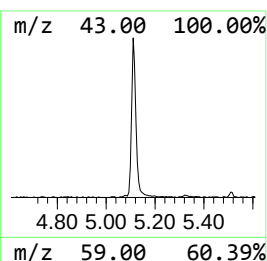
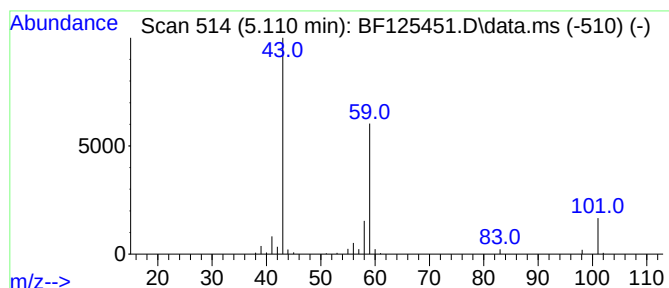
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	5.29 ng	260986	1,4-Dichlorobenzene-d4	6.887

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	47
3		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28



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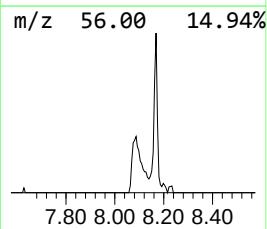
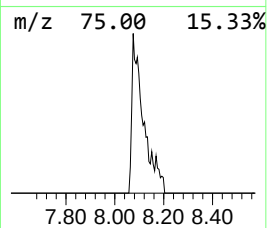
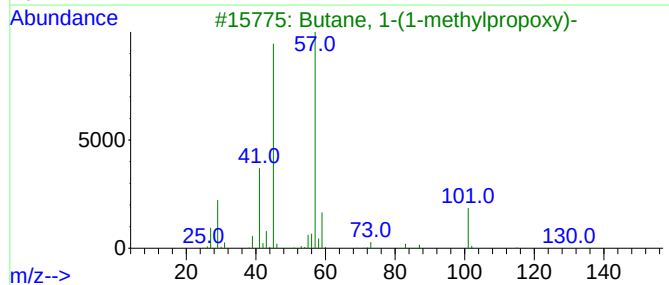
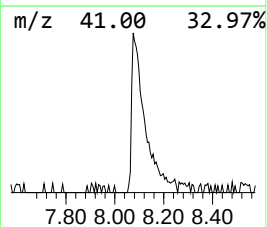
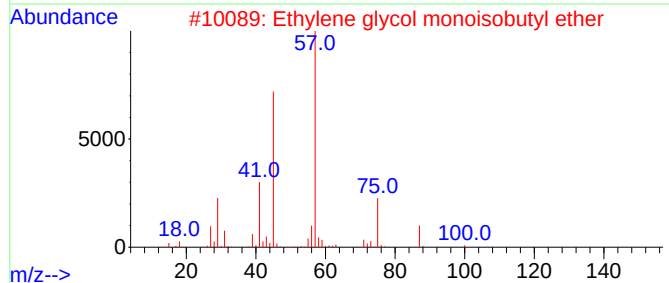
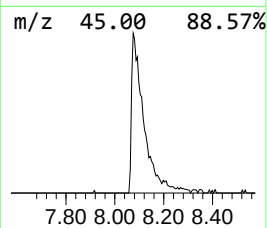
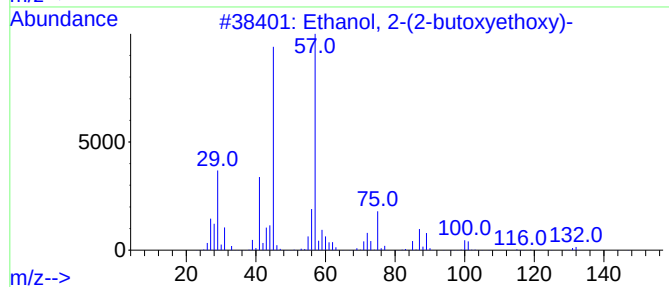
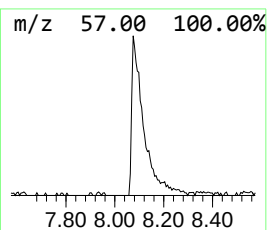
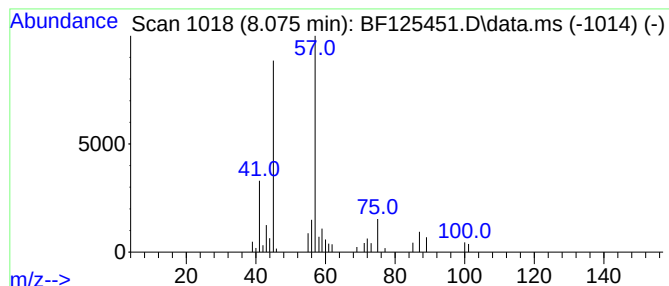
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	3.65 ng	249970	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	43
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	42



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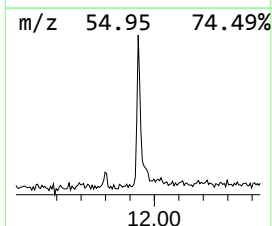
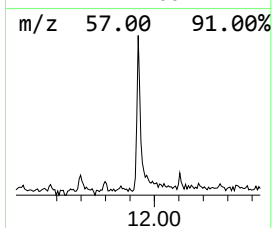
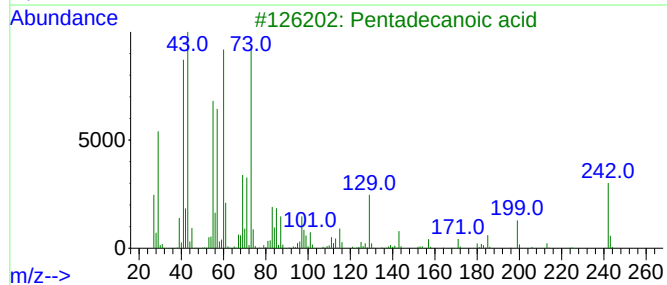
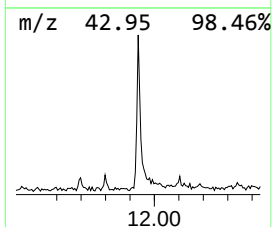
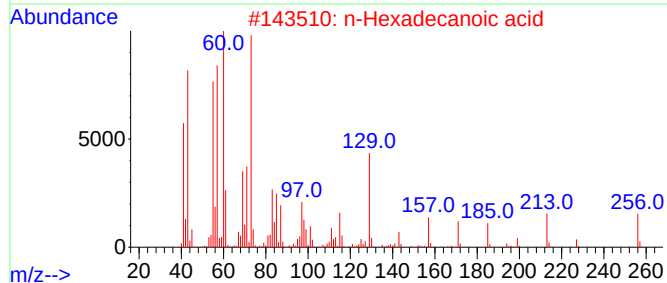
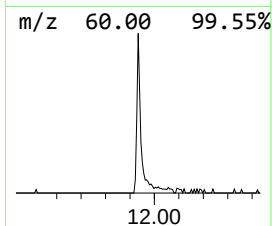
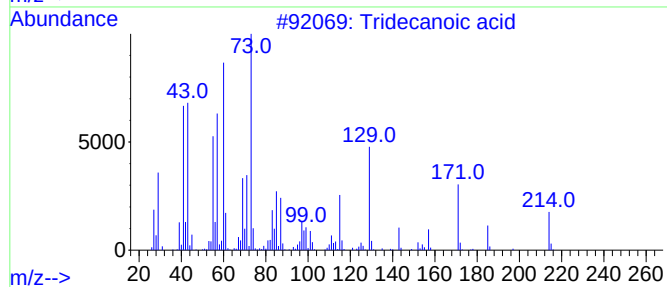
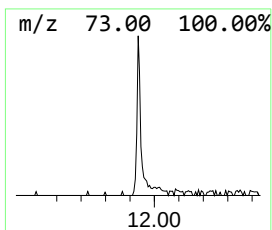
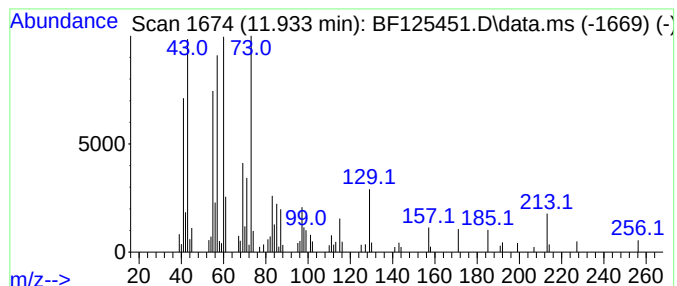
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.43 ng	188989	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	94
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Undecanoic acid	186	C11H22O2	000112-37-8	64



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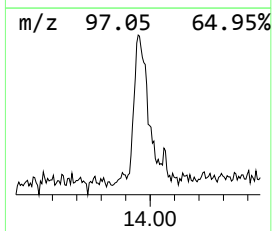
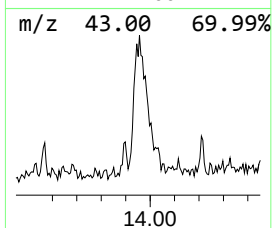
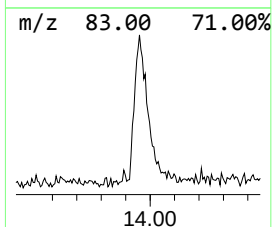
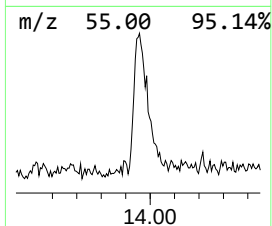
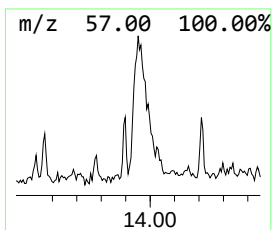
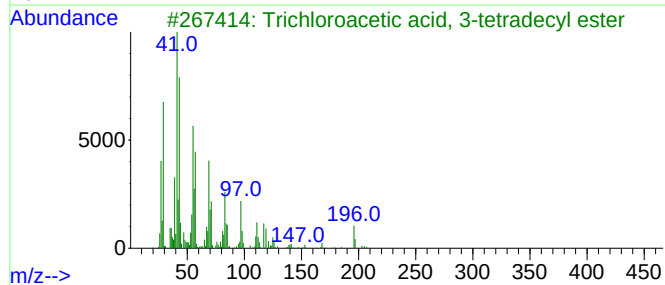
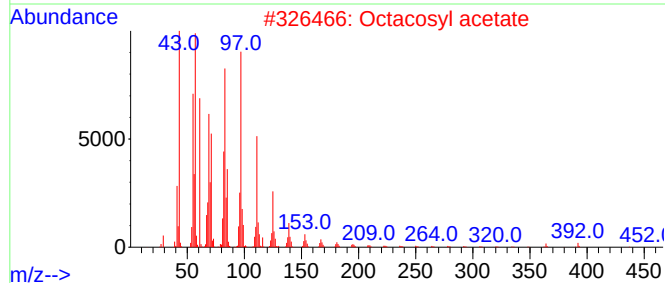
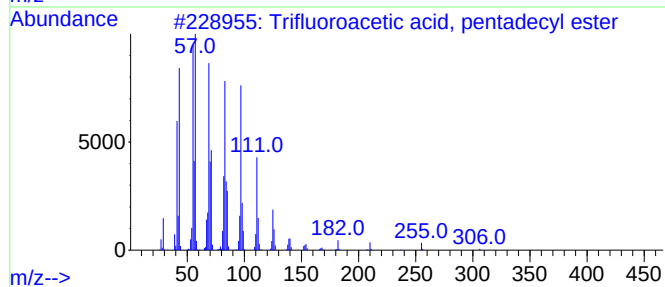
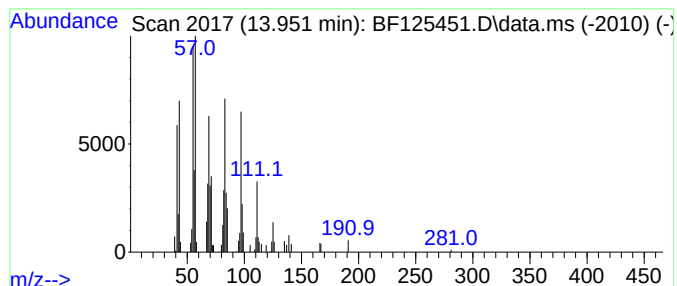
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Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.951	5.85 ng	306726	Chrysene-d12	14.063

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	90
2		Octacosyl acetate	452	C30H60O2	018206-97-8	87
3		Trichloroacetic acid, 3-tetradec...	358	C16H29Cl3O2	1000282-06-7	80
4		1-Heptadecene	238	C17H34	006765-39-5	80
5		1-Eicosene	280	C20H40	003452-07-1	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.193	42.6	ng	2103880	1	6.887	987012	20.0
2-Pentanone, 4-...	5.110	5.3	ng	260986	1	6.887	987012	20.0
Ethanol, 2-(2-b...	8.075	3.6	ng	249970	2	8.169	1369720	20.0
Tridecanoic acid	11.933	2.4	ng	188989	4	11.416	1554830	20.0
Trifluoroacetic...	13.951	5.8	ng	306726	5	14.063	1048380	20.0