

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
 Data File : BF096787.D
 Acq On : 14 Jul 2017 22:31
 Operator : SJ/JU
 Sample : I4176-06
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12003

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:\HPCHEM1\BNA_F\METHODS\8270-BF071317.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	4.804	475	479	489	rVB	152607	215898	8.38%	1.024%
2	5.239	548	553	562	rBV	2162087	2160005	83.86%	10.247%
3	6.275	724	729	732	rBV	2110949	2180315	84.64%	10.343%
4	6.398	745	750	753	rBV	2356401	2131515	82.75%	10.111%
5	6.622	785	788	792	rBV	668214	575148	22.33%	2.728%
6	6.781	811	815	818	rBV	1885967	1637883	63.59%	7.770%
7	7.186	879	884	887	rBV	1452517	1359287	52.77%	6.448%
8	7.904	1002	1006	1010	rBV	948838	873052	33.89%	4.142%
9	8.986	1184	1190	1193	rBV	2734711	2575866	100.00%	12.219%
10	9.380	1253	1257	1260	rBV	130198	113499	4.41%	0.538%
11	9.657	1299	1304	1308	rBV	894315	829556	32.20%	3.935%
12	9.874	1336	1341	1347	rBV2	29609	44620	1.73%	0.212%
13	10.104	1377	1380	1384	rVB	33134	26855	1.04%	0.127%
14	10.445	1433	1438	1441	rBV	1327494	1328490	51.57%	6.302%
15	10.574	1457	1460	1467	rBV	43506	48846	1.90%	0.232%
16	10.716	1473	1484	1491	rBV2	23063	60999	2.37%	0.289%
17	11.133	1551	1555	1558	rVB	967481	794357	30.84%	3.768%
18	11.680	1645	1648	1651	rBV	50241	47373	1.84%	0.225%
19	12.557	1795	1797	1801	rBV3	24135	28938	1.12%	0.137%
20	12.721	1820	1825	1828	rVB	2152408	2053383	79.72%	9.741%
21	13.627	1973	1979	1984	rBV	165966	204772	7.95%	0.971%
22	13.757	1997	2001	2005	rBV	725596	718522	27.89%	3.409%
23	14.409	2101	2112	2114	rBV4	206831	595430	23.12%	2.825%
24	15.139	2232	2236	2241	rBV	426951	475498	18.46%	2.256%

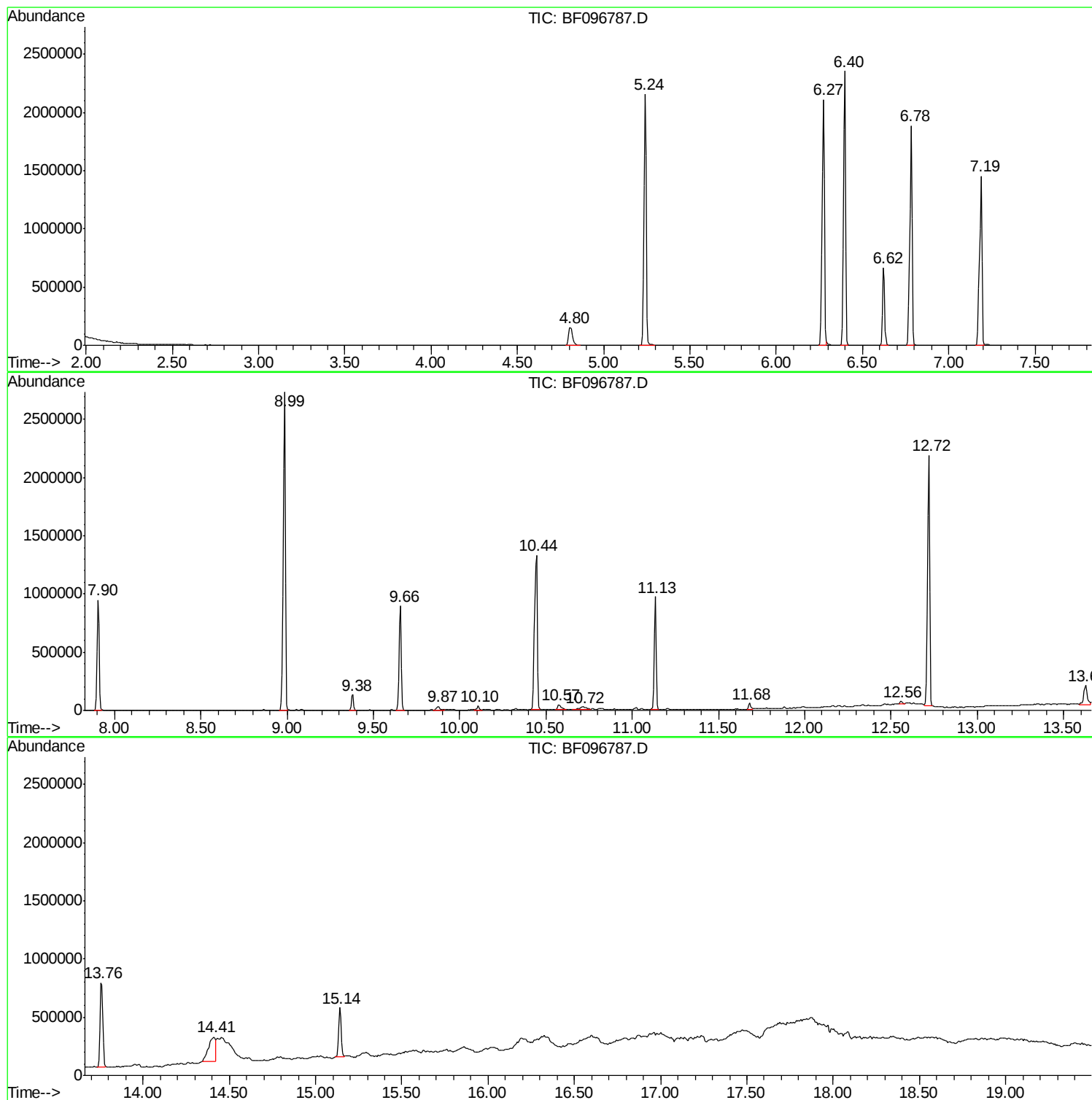
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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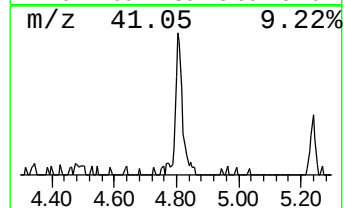
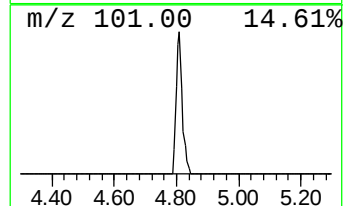
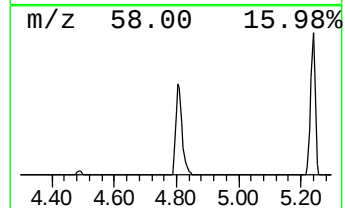
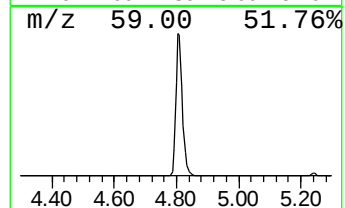
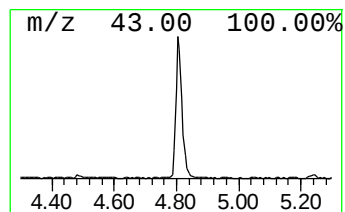
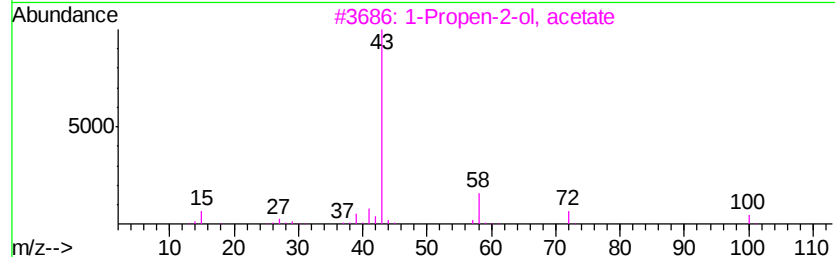
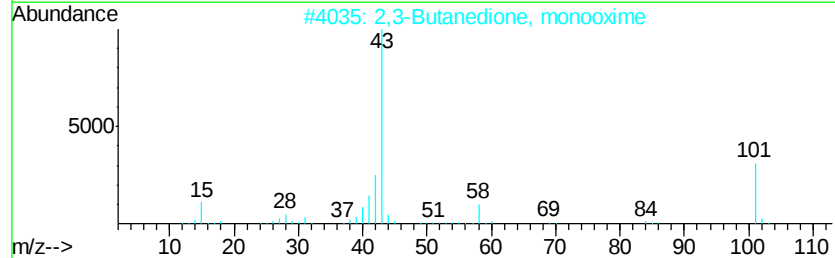
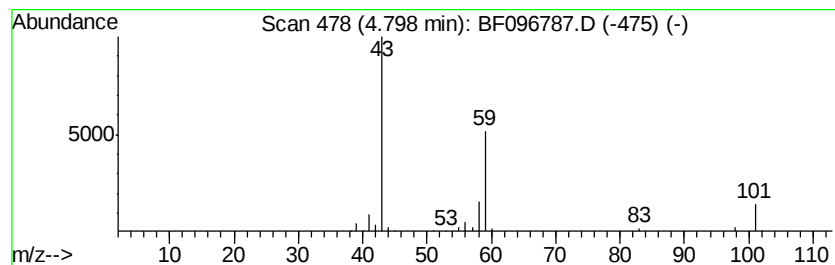
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.80	7.51 ng	215898	1,4-Dichlorobenzene-d4	6.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9	
4	4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	7	
5	Formamide, N,N-diethyl-	101	C5H11NO	000617-84-5	7	



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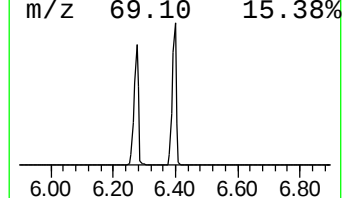
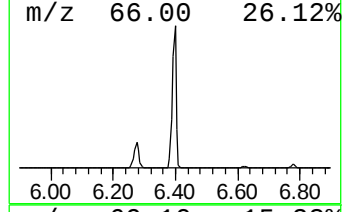
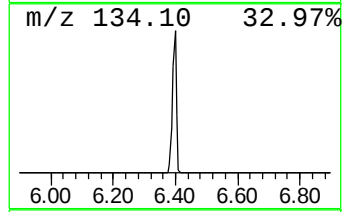
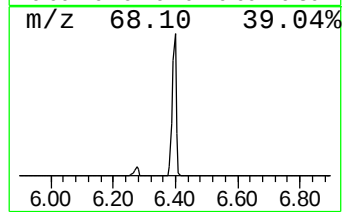
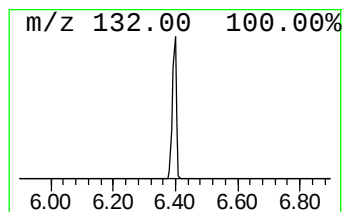
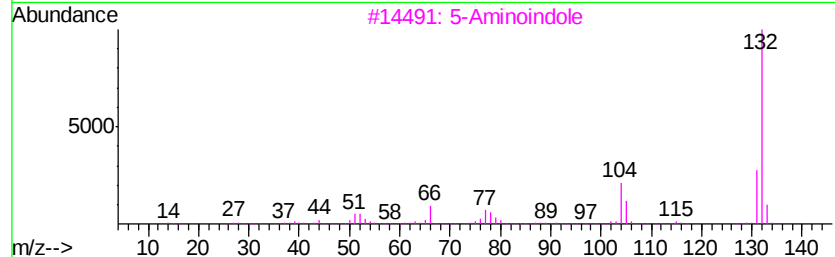
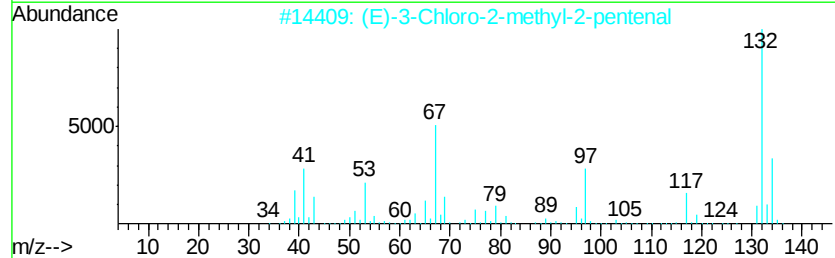
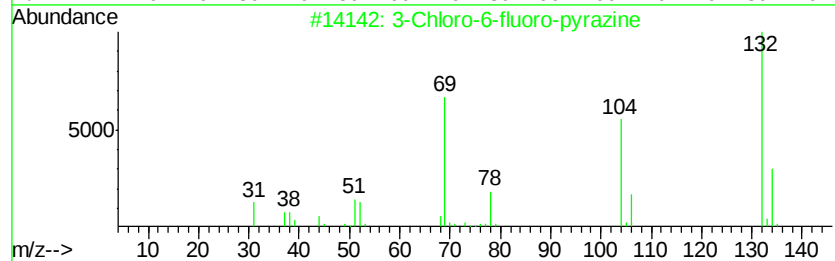
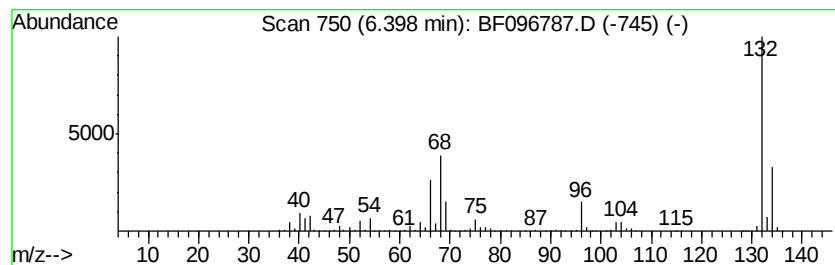
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Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	74.12 ng	2131520	1,4-Dichlorobenzene-d4	6.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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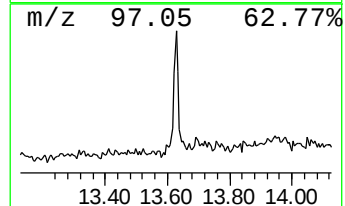
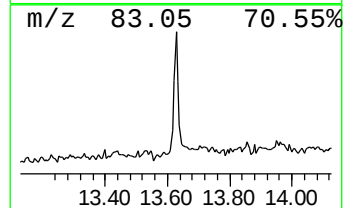
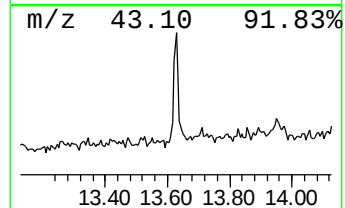
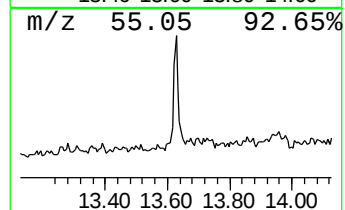
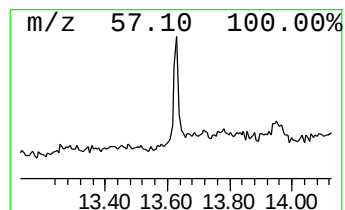
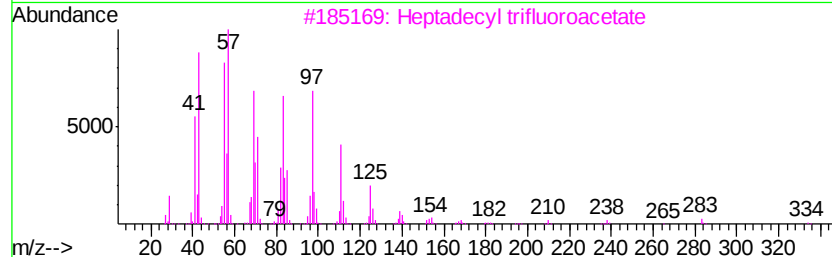
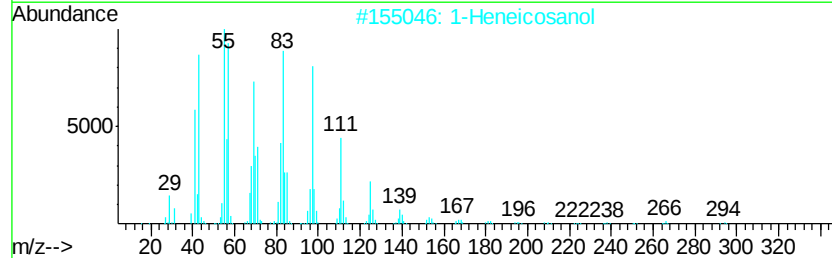
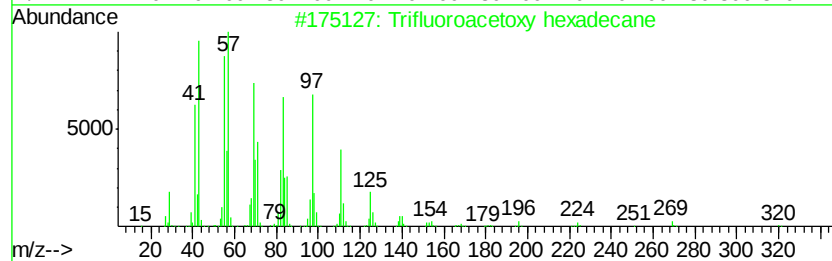
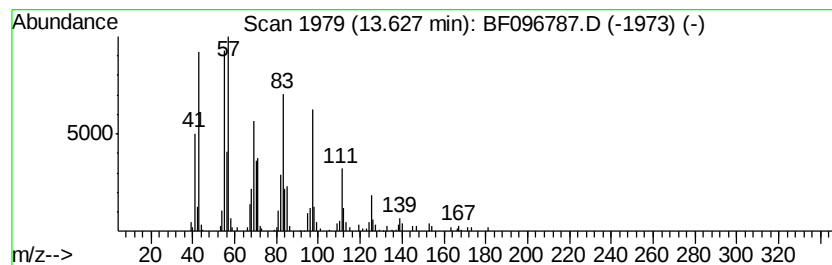
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.63	5.70 ng	204772	Chrysene-d12	13.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4		n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5		1-Nonadecene	266	C19H38	018435-45-5	91



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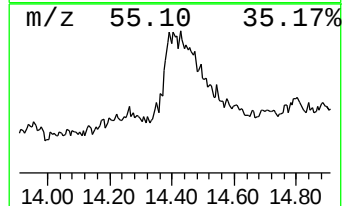
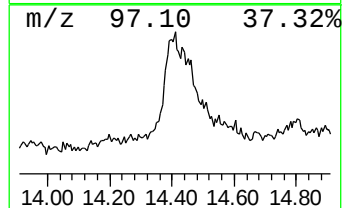
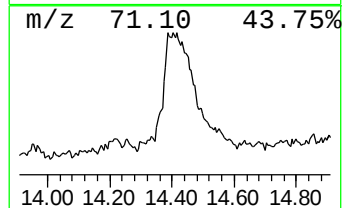
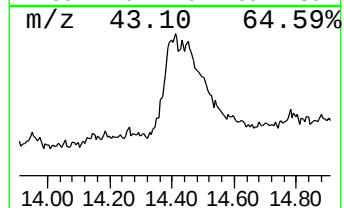
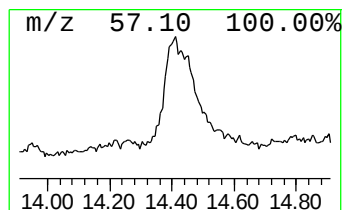
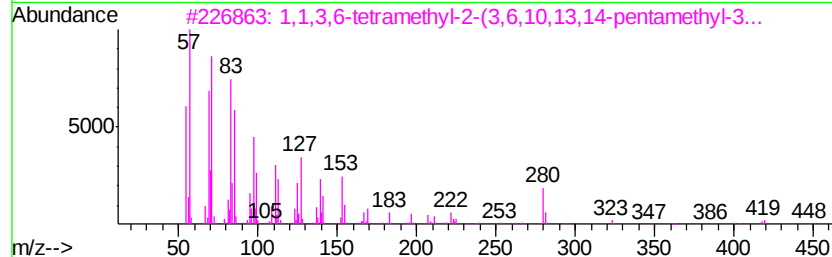
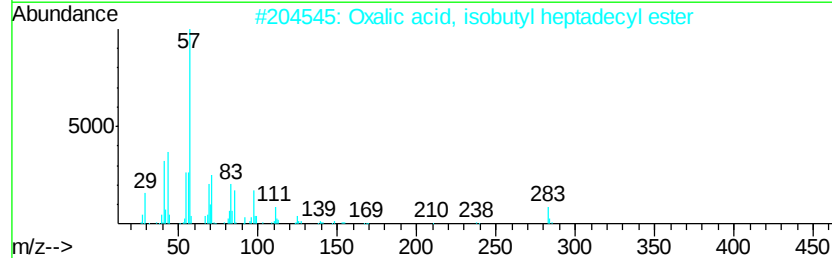
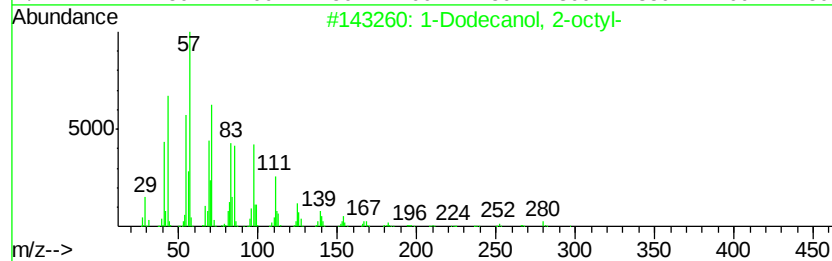
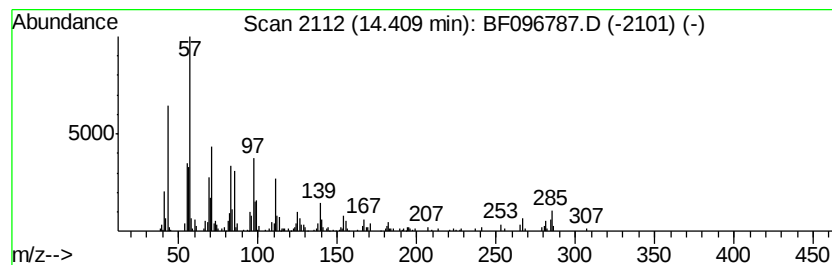
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Peak Number 5 1-Dodecanol, 2-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.41	16.57 ng	595430	Chrysene-d12	13.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	81
2		Oxalic acid, isobutyl heptadecyl...	384	C23H44O4	1000309-38-2	74
3		1,1,3,6-tetramethyl-2-(3,6,10,13...	449	C32H64	1000373-94-3	72
4		1-Decanol, 2-octyl-	270	C18H38O	045235-48-1	72
5		Octacosyl trifluoroacetate	506	C30H57F3O2	1000351-74-9	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	7.5	ng	215898	1	6.62	575148	20.0
unknown6.40	6.40	74.1	ng	2131520	1	6.62	575148	20.0
Trifluoroacetoxy ...	13.63	5.7	ng	204772	5	13.76	718522	20.0
1-Dodecanol, 2-oc...	14.41	16.6	ng	595430	5	13.76	718522	20.0