

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030123\
 Data File : BF132596.D
 Acq On : 01 Mar 2023 17:47
 Operator : CG\JU
 Sample : 01739-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SAMPLE-2-COMP-2

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132596.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	446	450	460	rVB	1343902	1533836	45.16%	5.945%
2	5.628	513	517	530	rBV	3491779	3332362	98.12%	12.916%
3	6.628	682	687	690	rBV	3254792	3188327	93.88%	12.358%
4	7.004	747	751	754	rBV	1224372	1025101	30.18%	3.973%
5	7.563	842	846	849	rBV	2468784	2046917	60.27%	7.934%
6	8.287	966	969	972	rBV	1613556	1235277	36.37%	4.788%
7	9.363	1148	1152	1155	rBV	4185530	3396350	100.00%	13.164%
8	10.051	1265	1269	1272	rBV	1392971	1204980	35.48%	4.670%
9	10.763	1386	1390	1393	rBV	204472	176885	5.21%	0.686%
10	10.839	1399	1403	1417	rBV	1989027	1740738	51.25%	6.747%
11	11.545	1519	1523	1526	rBV	1226822	1066147	31.39%	4.132%
12	12.051	1606	1609	1615	rBV	179941	212169	6.25%	0.822%
13	13.133	1789	1793	1796	rBV	3332344	2880568	84.81%	11.165%
14	13.351	1827	1830	1833	rBV	48530	47097	1.39%	0.183%
15	13.692	1884	1888	1891	rBV	62988	56341	1.66%	0.218%
16	14.045	1941	1948	1963	rBV5	85412	325155	9.57%	1.260%
17	14.198	1970	1974	1982	rBV	1198931	1187436	34.96%	4.602%
18	14.339	1995	1998	2005	rBV	39039	44763	1.32%	0.173%
19	15.063	2118	2121	2124	rVB	53172	50311	1.48%	0.195%
20	15.757	2233	2239	2246	rBV	728691	1049632	30.90%	4.068%

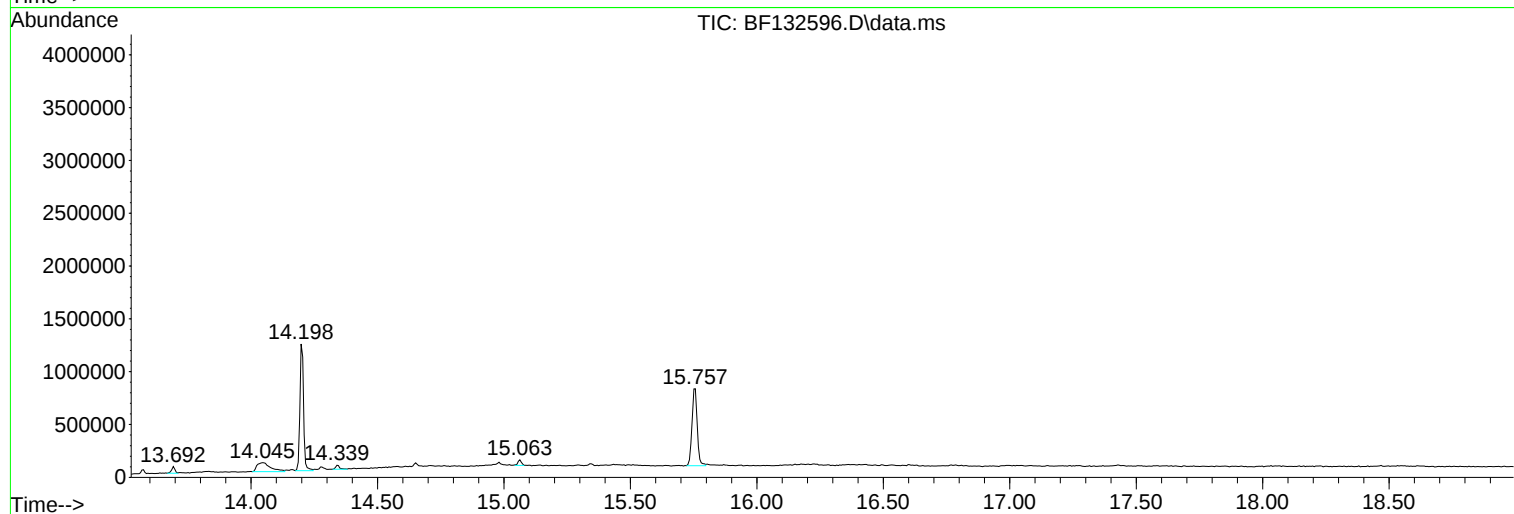
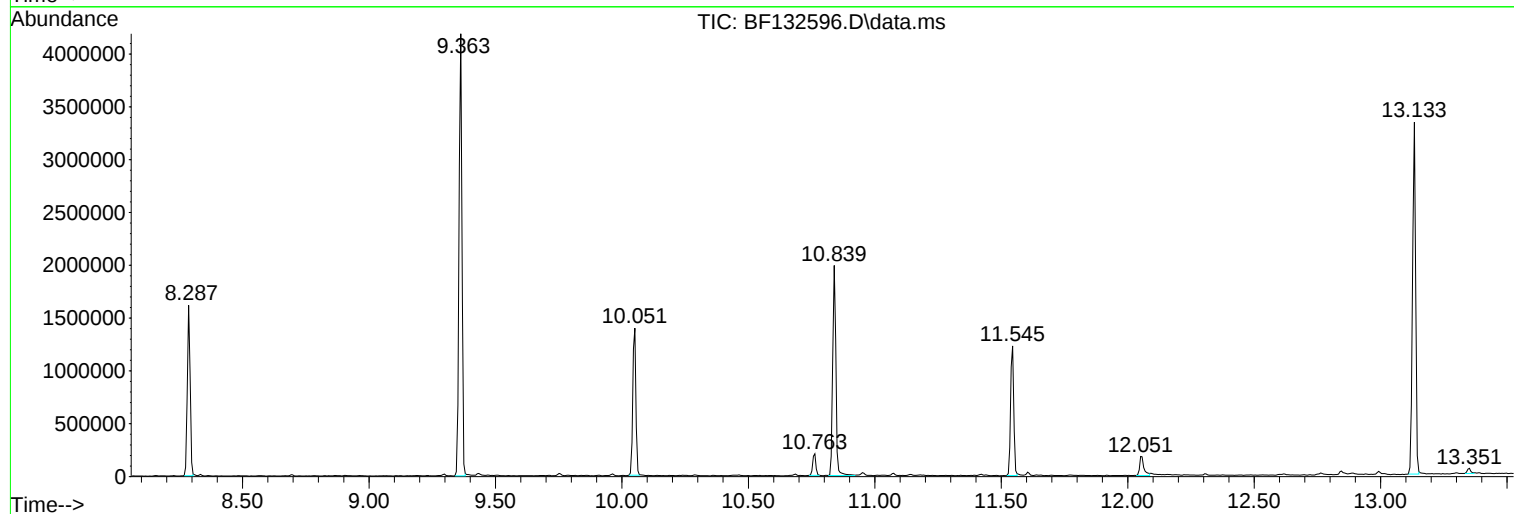
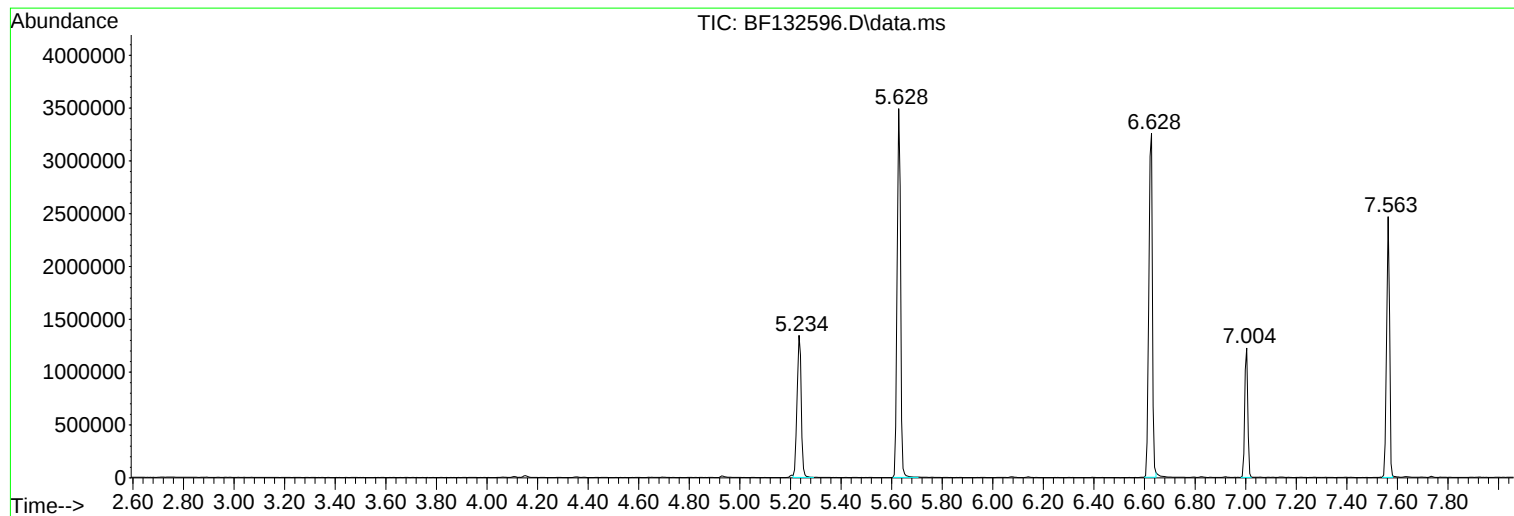
Sum of corrected areas: 25800392

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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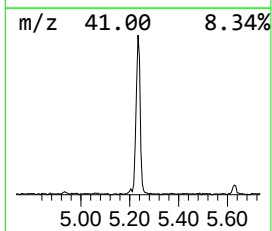
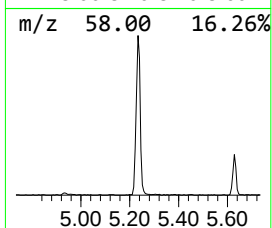
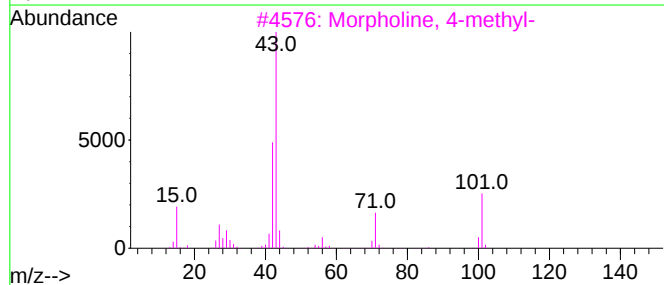
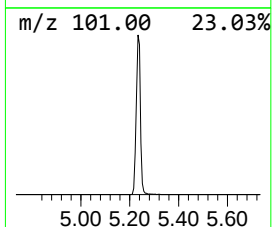
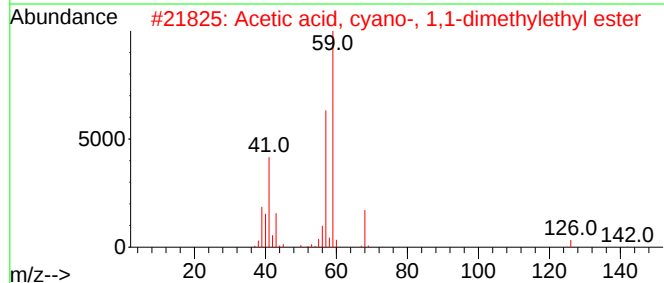
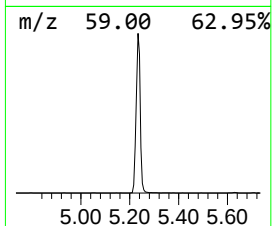
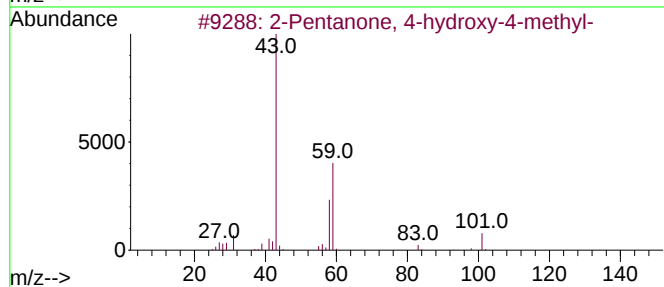
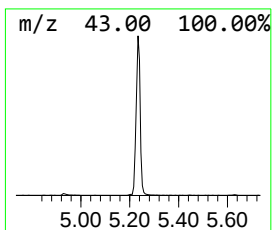
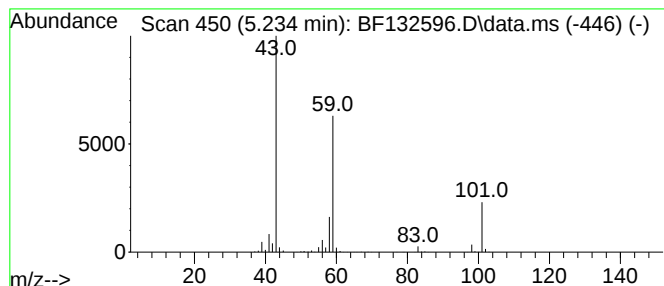
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.234	29.93 ng	1533840	1,4-Dichlorobenzene-d4	7.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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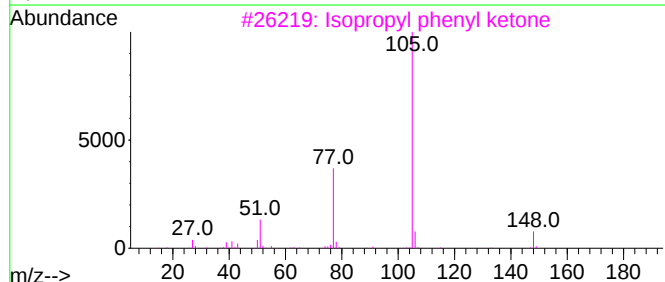
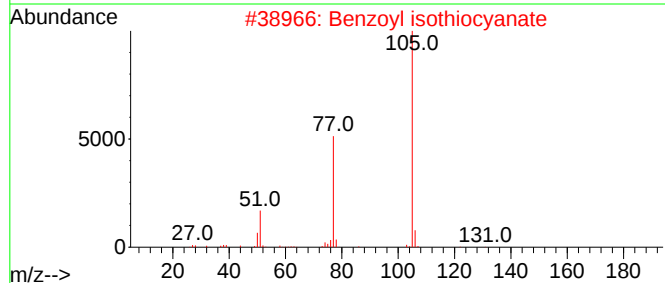
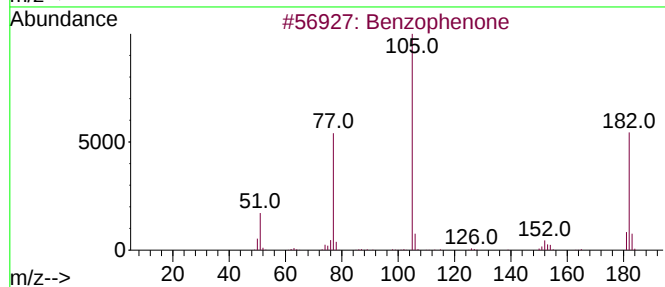
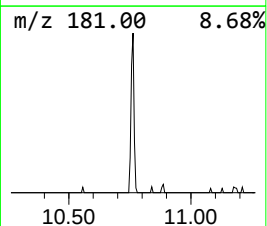
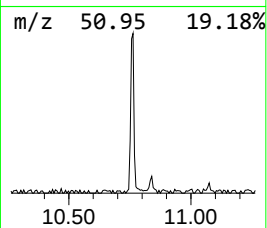
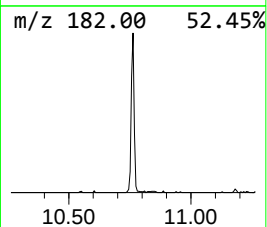
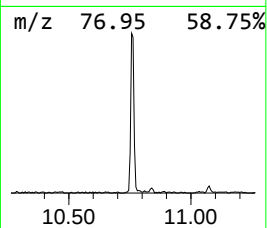
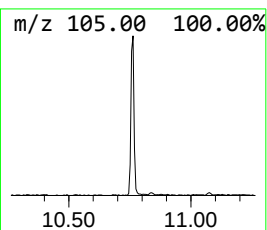
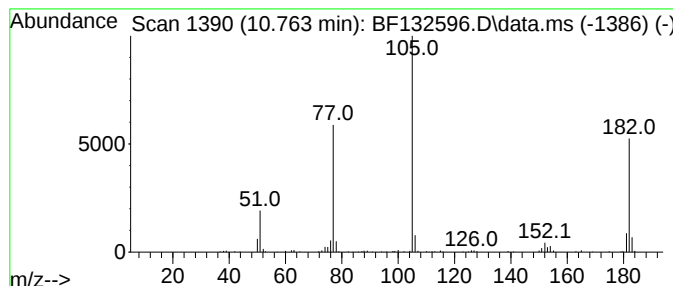
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	2.94 ng	176885	Acenaphthene-d10	10.051

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	49
3			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	47
4			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	47
5			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	47



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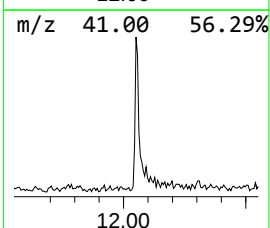
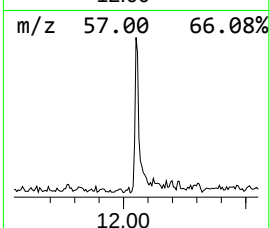
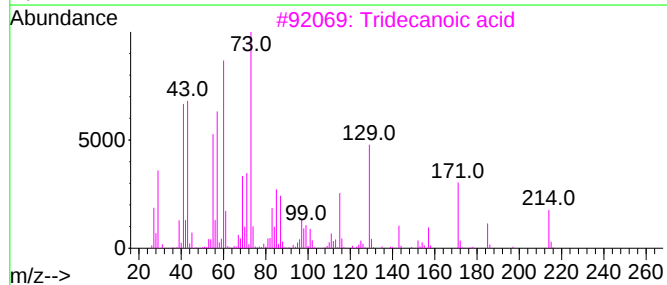
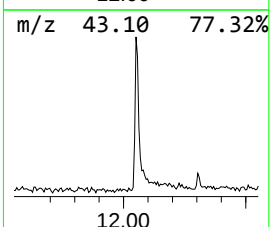
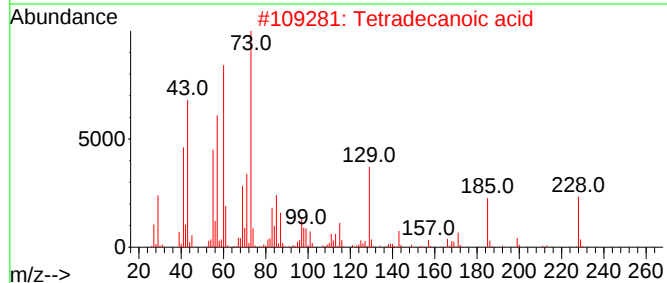
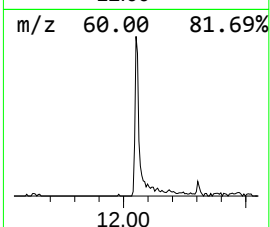
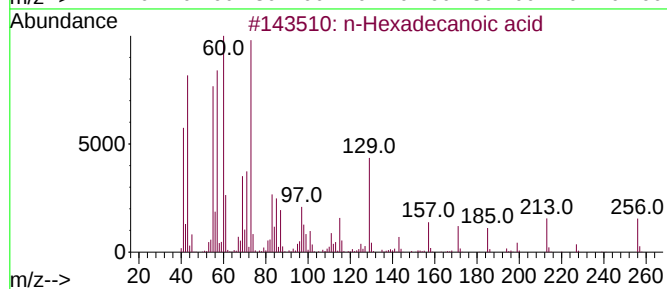
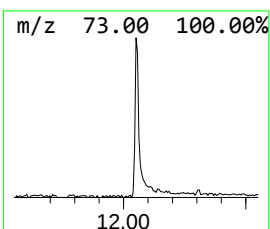
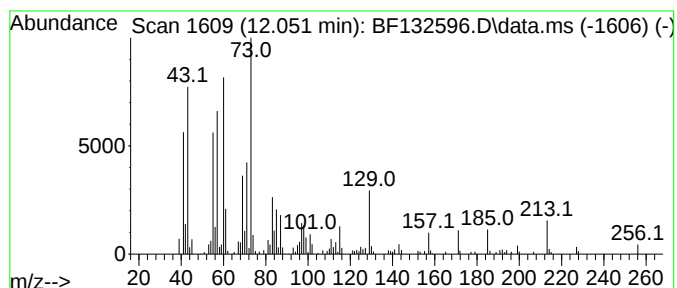
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.051	3.98 ng	212169	Phenanthrene-d10	11.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid			256	C16H32O2	000057-10-3	97
2	Tetradecanoic acid			228	C14H28O2	000544-63-8	94
3	Tridecanoic acid			214	C13H26O2	000638-53-9	93
4	Pentadecanoic acid			242	C15H30O2	001002-84-2	74
5	Dodecanoic acid			200	C12H24O2	000143-07-7	70



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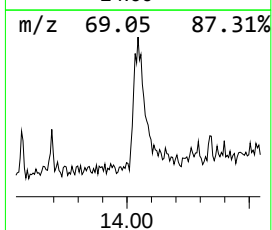
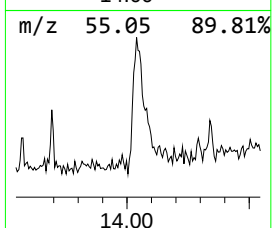
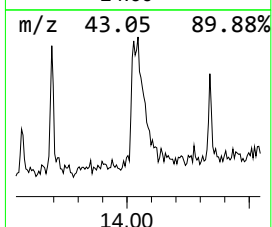
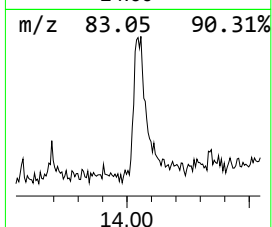
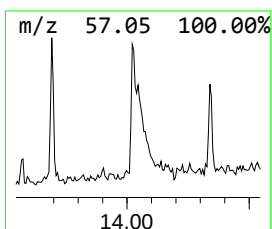
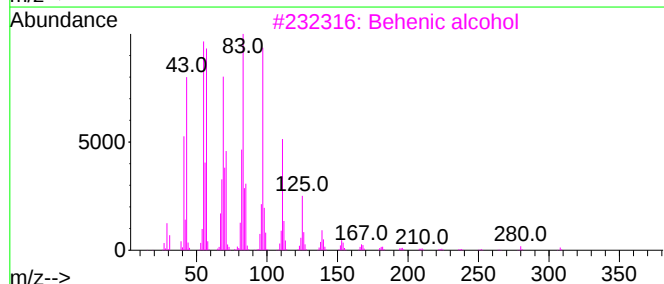
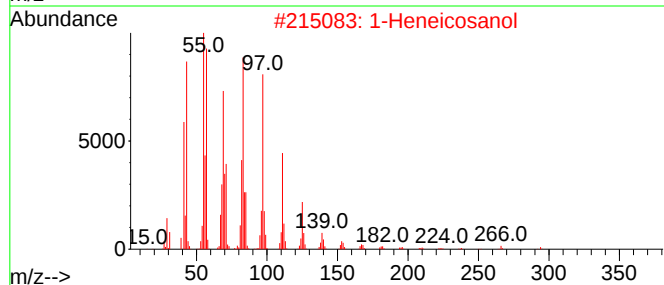
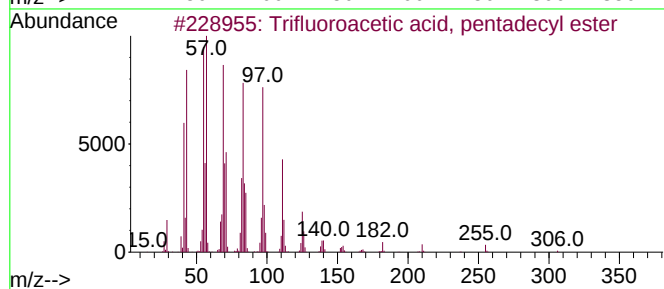
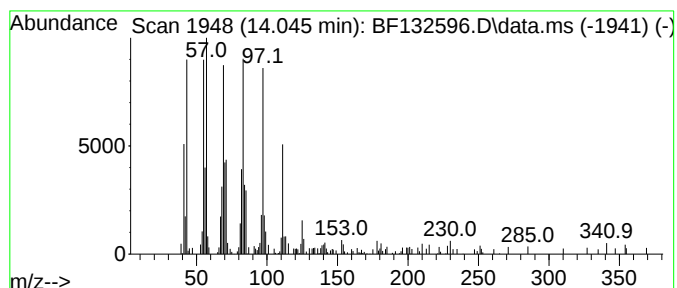
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetic acid, penta... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.045	5.48 ng	325155	Chrysene-d12	14.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	91
3			Behenic alcohol	326	C22H46O	000661-19-8	91
4			Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	91
5			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.234	29.9	ng	1533840	1	7.004	1025100	20.0
Benzophenone	10.763	2.9	ng	176885	3	10.051	1204980	20.0
n-Hexadecanoic ...	12.051	4.0	ng	212169	4	11.545	1066150	20.0
Trifluoroacetic...	14.045	5.5	ng	325155	5	14.198	1187440	20.0