

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF050721\
 Data File : BF123878.D
 Acq On : 7 May 2021 21:34
 Operator : JU/CG
 Sample : M2295-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 DRUM-D-E

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-BF042721.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	486	493	496	rVB	2383368	3108903	64.61%	10.037%
2	5.404	560	564	573	rBV	3402945	2982749	61.99%	9.630%
3	6.328	718	721	726	rBV	118420	123629	2.57%	0.399%
4	6.422	733	737	746	rVB	3545126	3995288	83.04%	12.898%
5	6.775	794	797	801	rBV	879599	677133	14.07%	2.186%
6	6.957	825	828	831	rVB	67814	54023	1.12%	0.174%
7	7.339	888	893	896	rBV	2447521	2375689	49.37%	7.670%
8	7.969	997	1000	1012	rBV	133242	169445	3.52%	0.547%
9	8.057	1012	1015	1017	rVV	1064220	888497	18.47%	2.868%
10	8.081	1017	1019	1022	rVB	467870	330778	6.87%	1.068%
11	8.775	1134	1137	1140	rVB	70961	56834	1.18%	0.183%
12	9.139	1194	1199	1202	rBV	5160449	4117165	85.57%	13.292%
13	9.533	1263	1266	1269	rBV	110285	89586	1.86%	0.289%
14	9.816	1310	1314	1317	rBV	1202916	945822	19.66%	3.054%
15	9.845	1317	1319	1323	rVB	87679	68108	1.42%	0.220%
16	10.604	1444	1448	1451	rBV	2898430	2381292	49.49%	7.688%
17	11.298	1563	1566	1569	rBV	1454384	1173508	24.39%	3.789%
18	11.322	1569	1570	1573	rVV	136812	81711	1.70%	0.264%
19	11.374	1573	1579	1582	rVB3	47560	53545	1.11%	0.173%
20	12.892	1832	1837	1840	rBV	4998980	4811545	100.00%	15.534%
21	13.815	1984	1994	2004	rBV5	100837	271866	5.65%	0.878%
22	13.939	2011	2015	2019	rBV	1188474	990963	20.60%	3.199%
23	15.380	2255	2260	2265	rBV	668482	875090	18.19%	2.825%
24	15.839	2332	2338	2342	rBV2	50106	74601	1.55%	0.241%
25	16.321	2416	2420	2424	rBV3	47369	79096	1.64%	0.255%
26	16.904	2513	2519	2528	rVB7	35234	77791	1.62%	0.251%
27	17.580	2628	2634	2641	rBV9	25114	63819	1.33%	0.206%
28	18.392	2763	2772	2775	rBV10	20315	56533	1.17%	0.183%

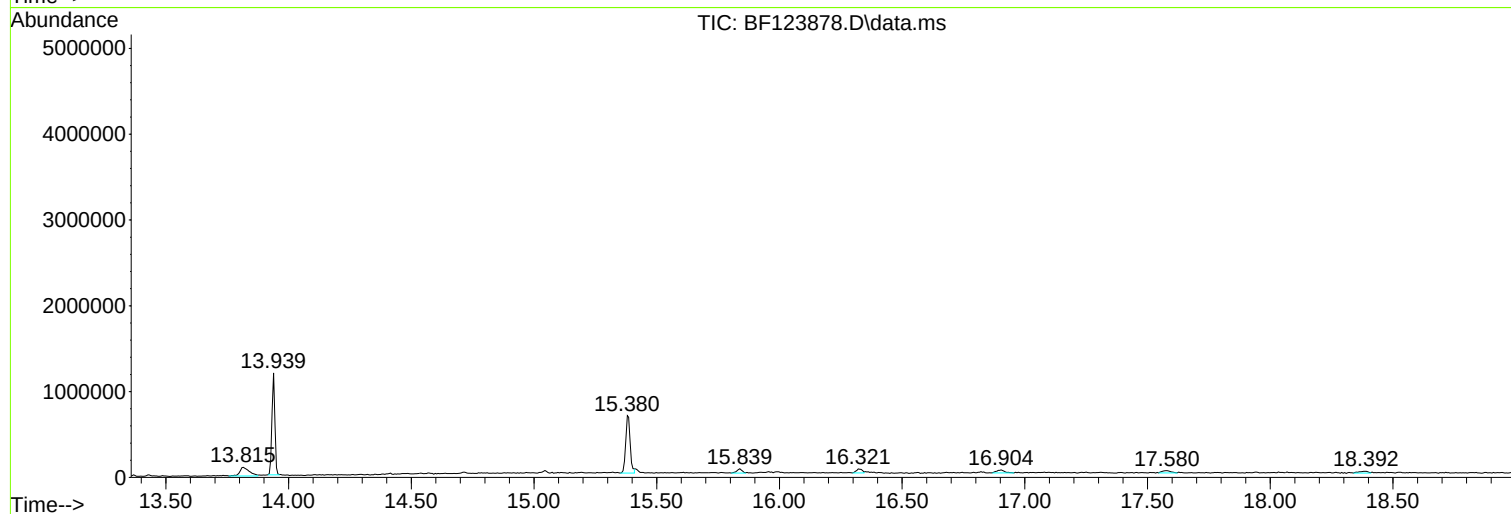
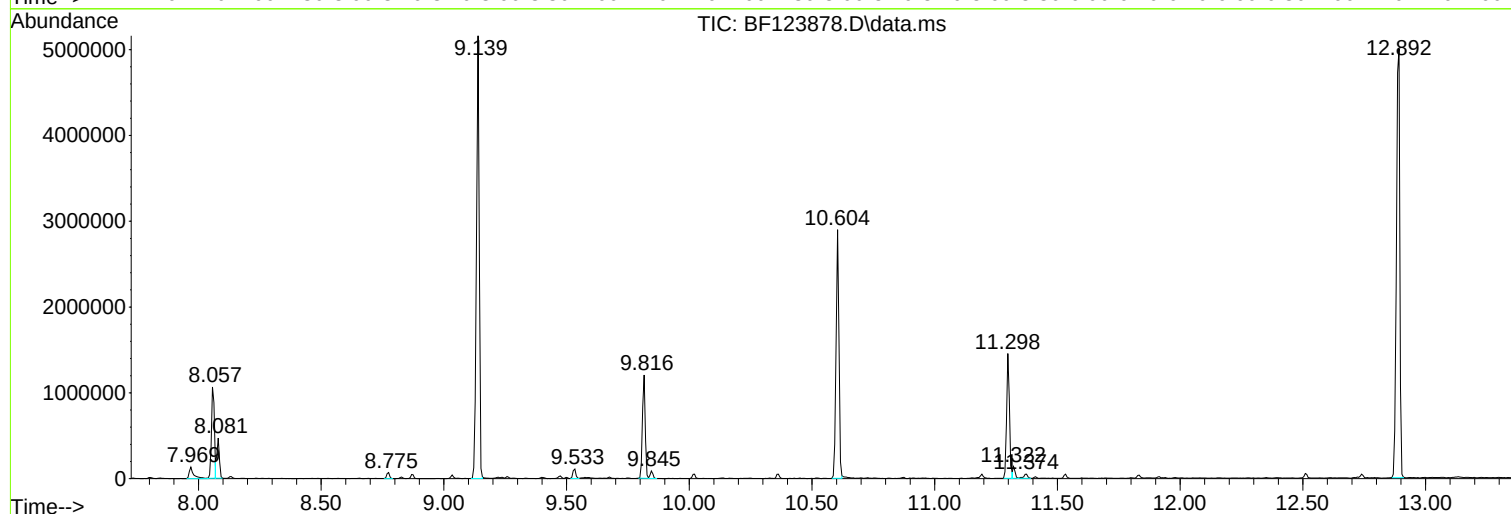
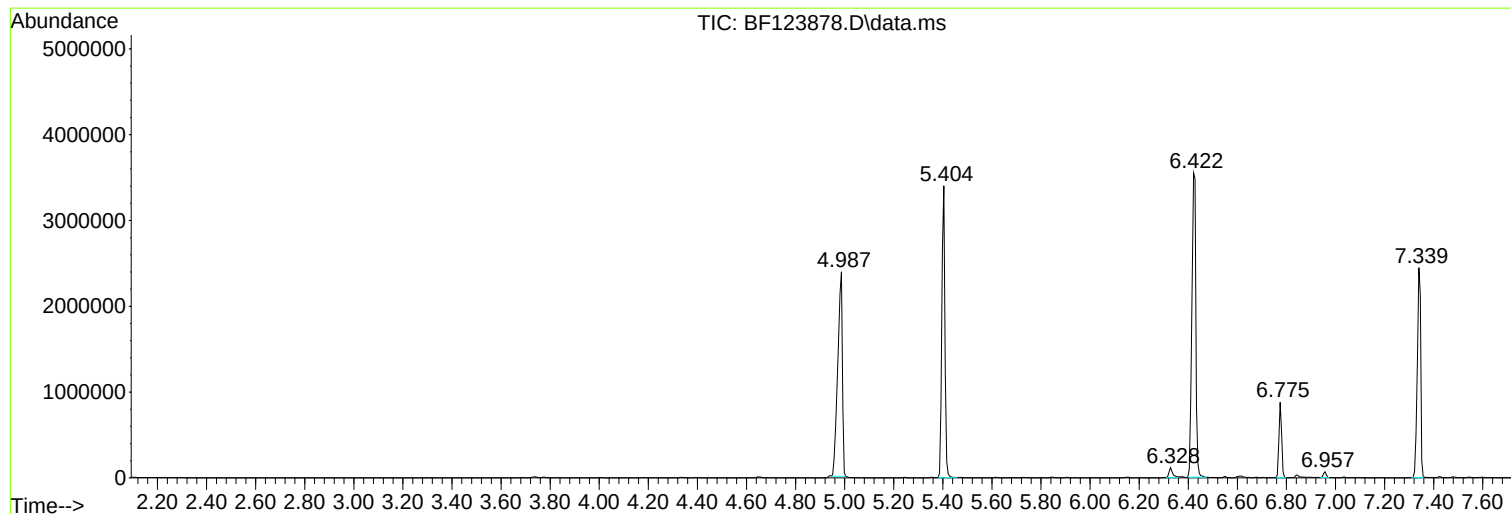
Sum of corrected areas: 30975009

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.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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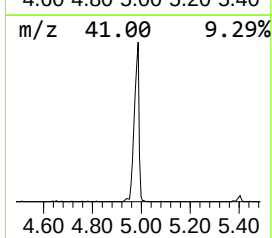
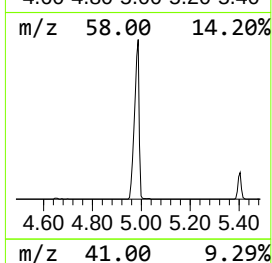
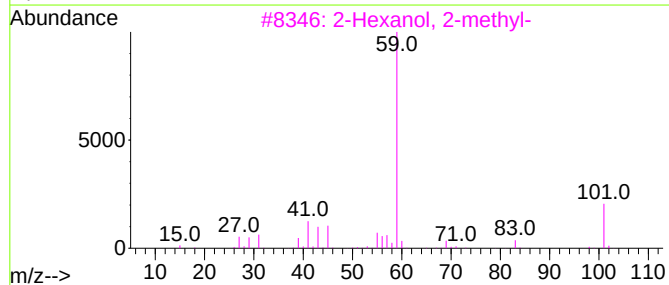
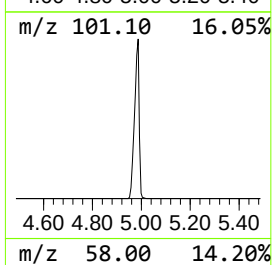
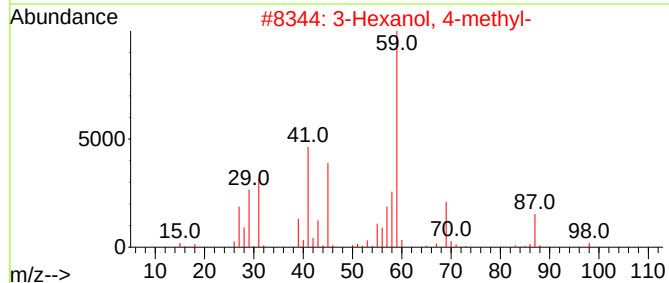
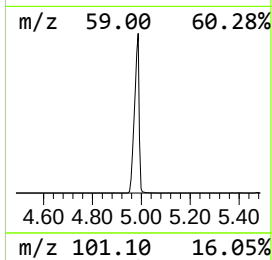
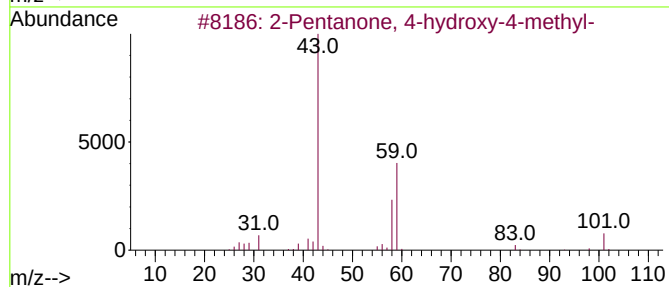
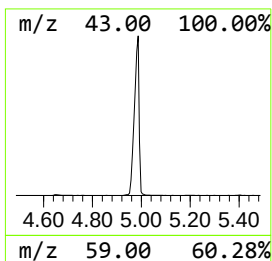
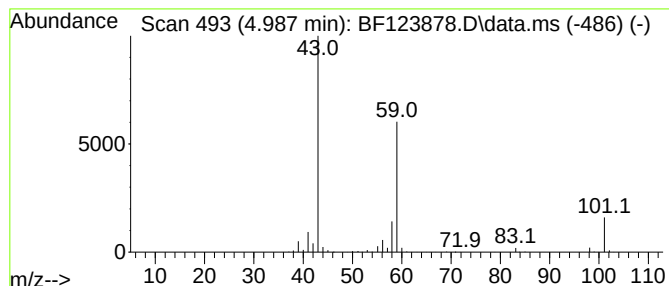
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF042721.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.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.
4.987	91.83 ng	3108900	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28		
5	3-Pentanol	88	C5H12O	000584-02-1	9		



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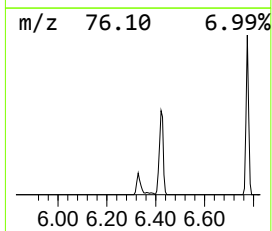
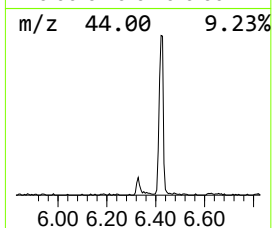
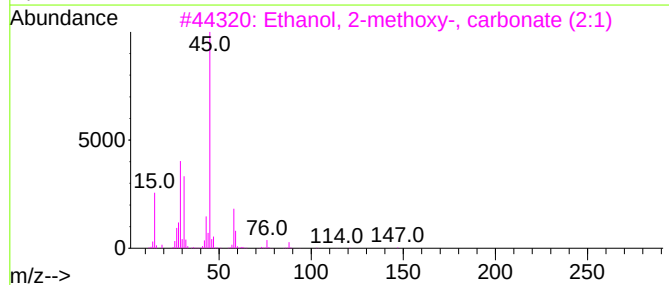
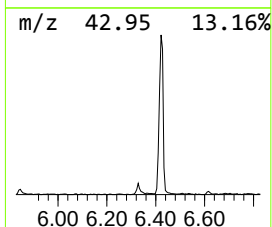
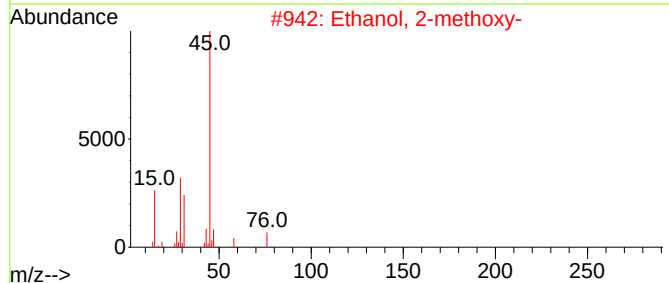
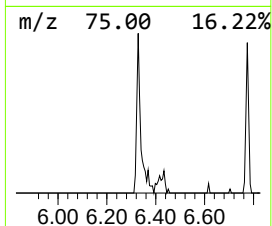
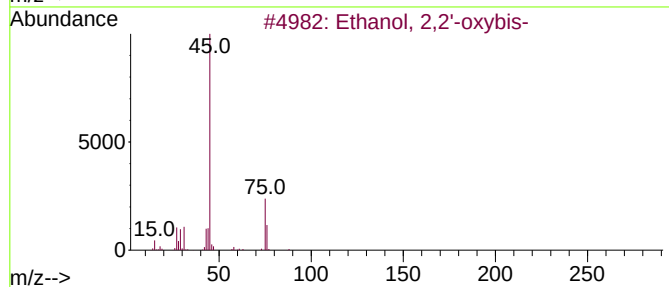
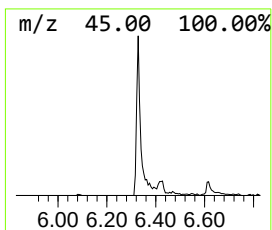
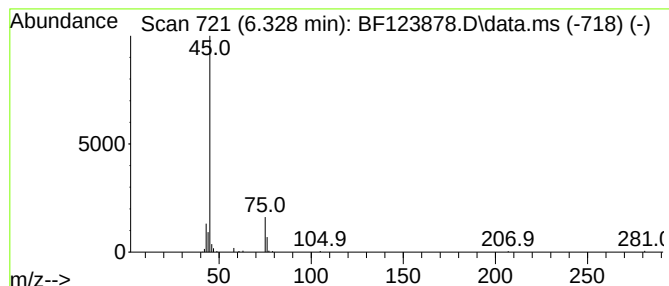
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.328	3.65 ng	123629	1,4-Dichlorobenzene-d4	6.775

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	78
2			Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
3			Ethanol, 2-methoxy-, carbonate (...)	178	C7H14O5	000626-84-6	9
4			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	9
5			2-Butanol, (R)-	74	C4H10O	014898-79-4	9



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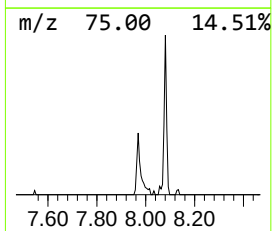
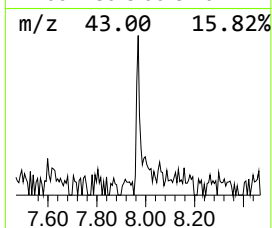
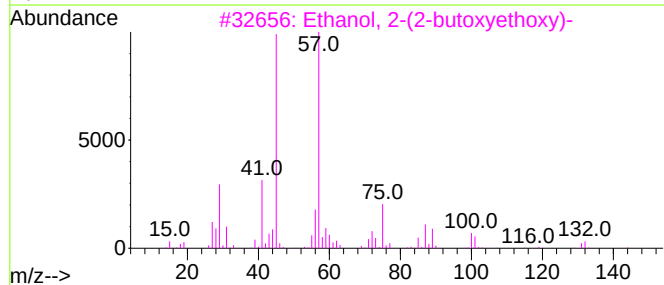
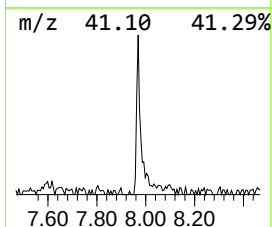
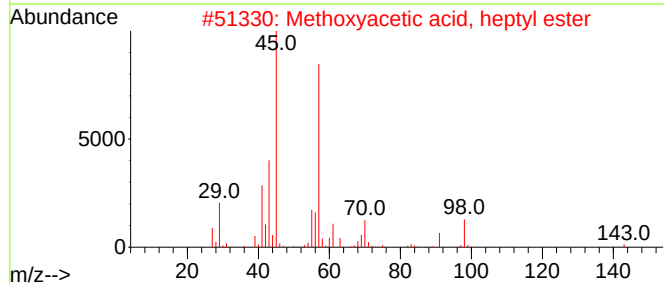
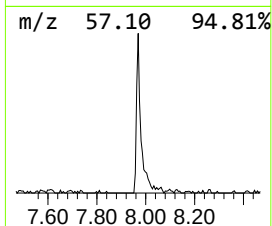
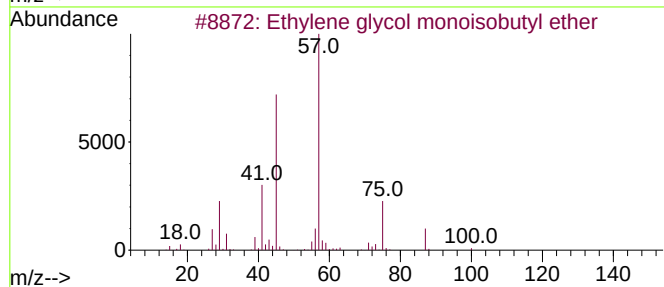
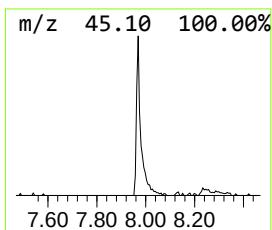
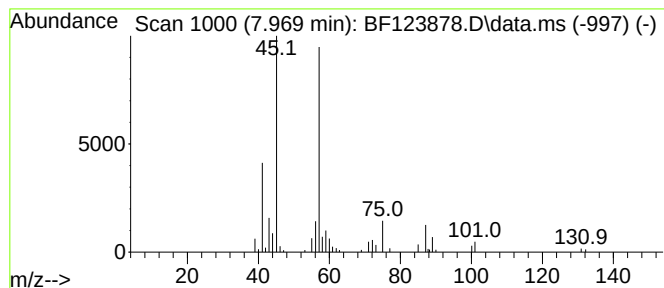
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Peak Number 3 Ethylene glycol monoisobuty... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.969	3.81 ng	169445	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
2			Methoxyacetic acid, heptyl ester	188	C10H20O3	168920-36-3	50
3			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	47
4			2-Pentanol, 3-methyl-	102	C6H14O	000565-60-6	43
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	43



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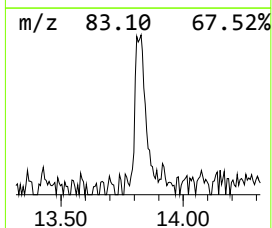
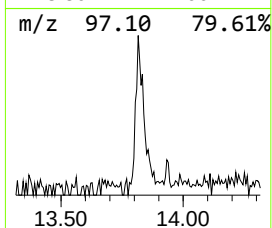
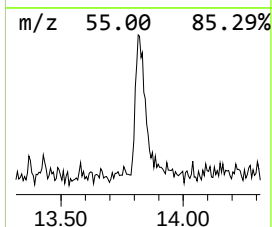
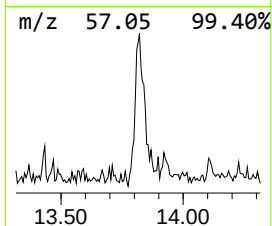
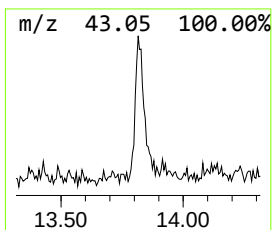
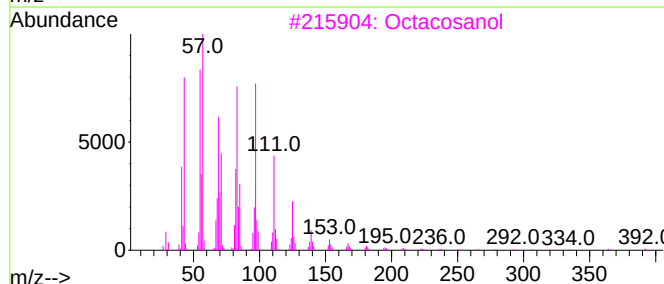
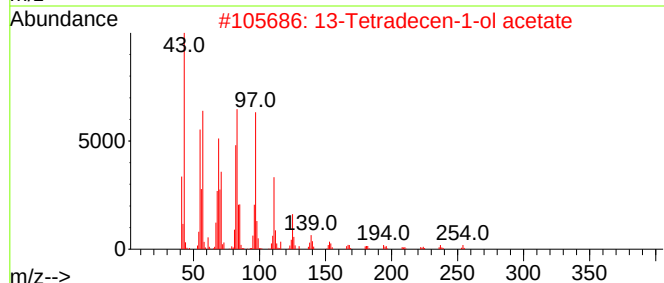
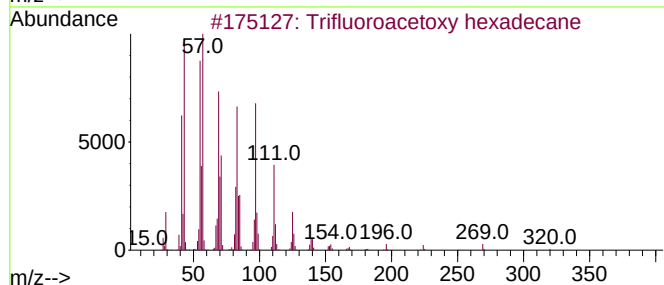
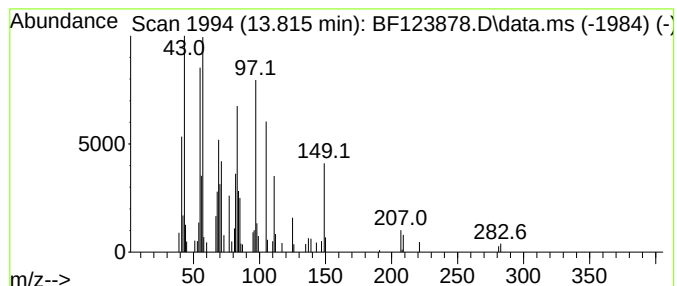
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.816	5.49 ng	271866	Chrysene-d12	13.939	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	74
2	13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	74
3	Octacosanol	410	C28H58O	000557-61-9	68
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	60
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	60



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	91.8	ng	3108900	1	6.775	677133	20.0
Ethanol, 2,2'-o...	6.328	3.6	ng	123629	1	6.775	677133	20.0
Ethylene glycol...	7.969	3.8	ng	169445	2	8.057	888497	20.0
Trifluoroacetox...	13.816	5.5	ng	271866	5	13.939	990963	20.0