

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF102621\
 Data File : BF125938.D
 Acq On : 26 Oct 2021 17:22
 Operator : JU/CG
 Sample : M4340-04
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TH-ED

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-BF102521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125938.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	7	14	24	rVB	2379570	3209114	71.33%	8.746%
2	3.357	213	216	228	rBV2	23757	59913	1.33%	0.163%
3	5.481	572	577	580	rBV	4195026	4414114	98.11%	12.031%
4	6.487	742	748	751	rBV	4018213	4499254	100.00%	12.263%
5	6.692	781	783	788	rBV	57726	46826	1.04%	0.128%
6	6.863	809	812	816	rBV	1226205	1060569	23.57%	2.891%
7	7.428	902	908	911	rBV	3005369	2920686	64.91%	7.960%
8	8.051	1010	1014	1017	rBV	1601921	1307974	29.07%	3.565%
9	8.145	1026	1030	1034	rVB	1575729	1376349	30.59%	3.751%
10	9.228	1209	1214	1217	rBV	4275663	4212407	93.62%	11.481%
11	9.904	1324	1329	1332	rVB	1678912	1516351	33.70%	4.133%
12	10.310	1392	1398	1409	rVB	165845	195576	4.35%	0.533%
13	10.686	1458	1462	1465	rBV	3361273	3002975	66.74%	8.185%
14	11.386	1577	1581	1584	rBV	1924753	1559737	34.67%	4.251%
15	11.451	1587	1592	1595	rBV5	43892	49103	1.09%	0.134%
16	11.786	1643	1649	1652	rVB2	92775	120084	2.67%	0.327%
17	11.916	1665	1671	1675	rBV	357034	373173	8.29%	1.017%
18	12.698	1799	1804	1811	rBV2	106985	140350	3.12%	0.383%
19	12.974	1847	1851	1854	rBV	4278835	3868942	85.99%	10.545%
20	13.521	1940	1944	1948	rBV3	43645	60891	1.35%	0.166%
21	13.874	2000	2004	2011	rBV	296124	319561	7.10%	0.871%
22	14.021	2025	2029	2033	rBV	1182722	1022084	22.72%	2.786%
23	14.510	2109	2112	2115	rBV	116524	102581	2.28%	0.280%
24	14.898	2175	2178	2182	rVB2	74386	87172	1.94%	0.238%
25	15.162	2220	2223	2231	rBV6	50953	81900	1.82%	0.223%
26	15.492	2274	2279	2286	rBV	811458	941185	20.92%	2.565%
27	15.992	2360	2364	2368	rBV5	37427	60402	1.34%	0.165%
28	16.033	2368	2371	2378	rVB5	51629	81250	1.81%	0.221%

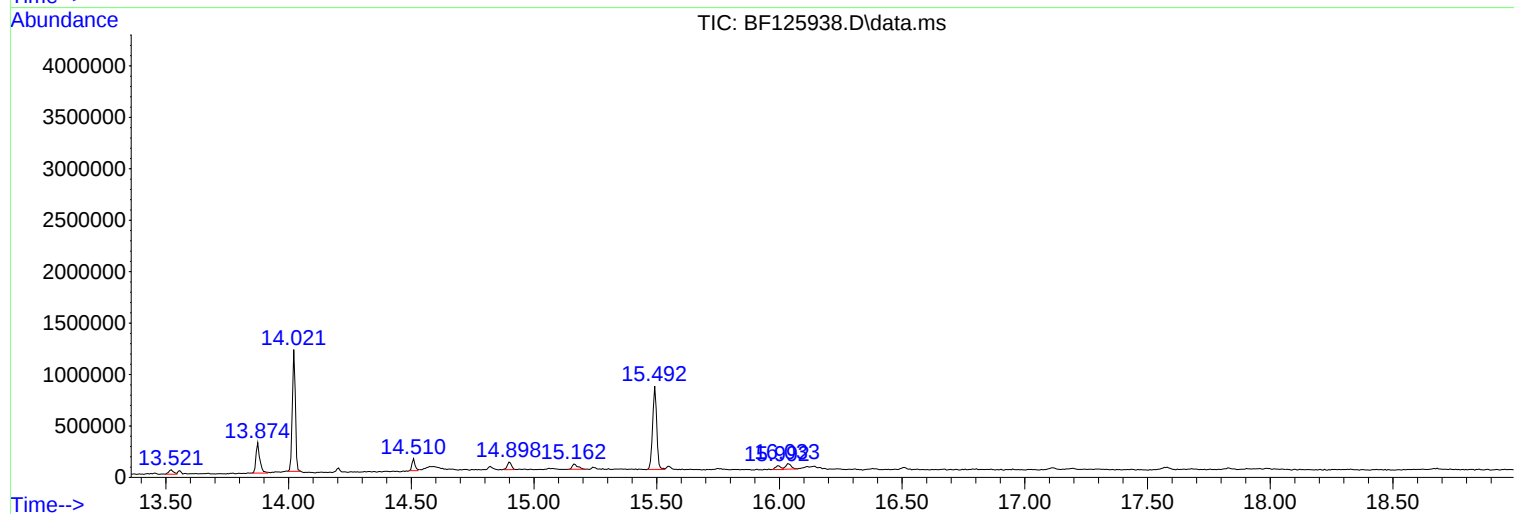
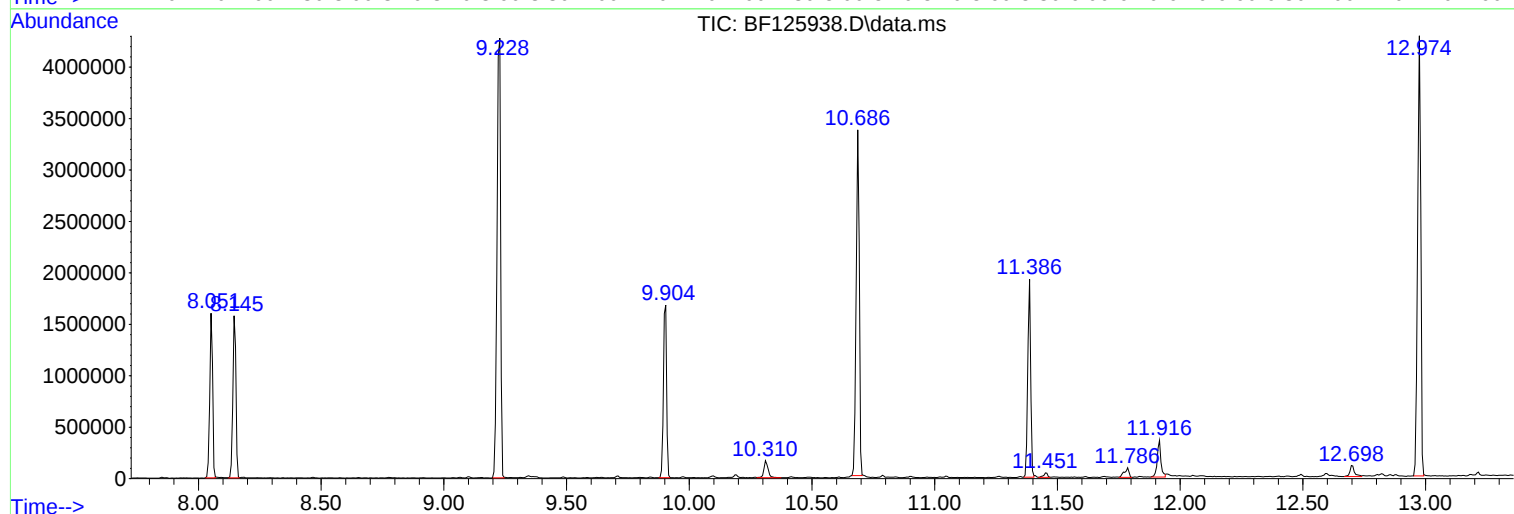
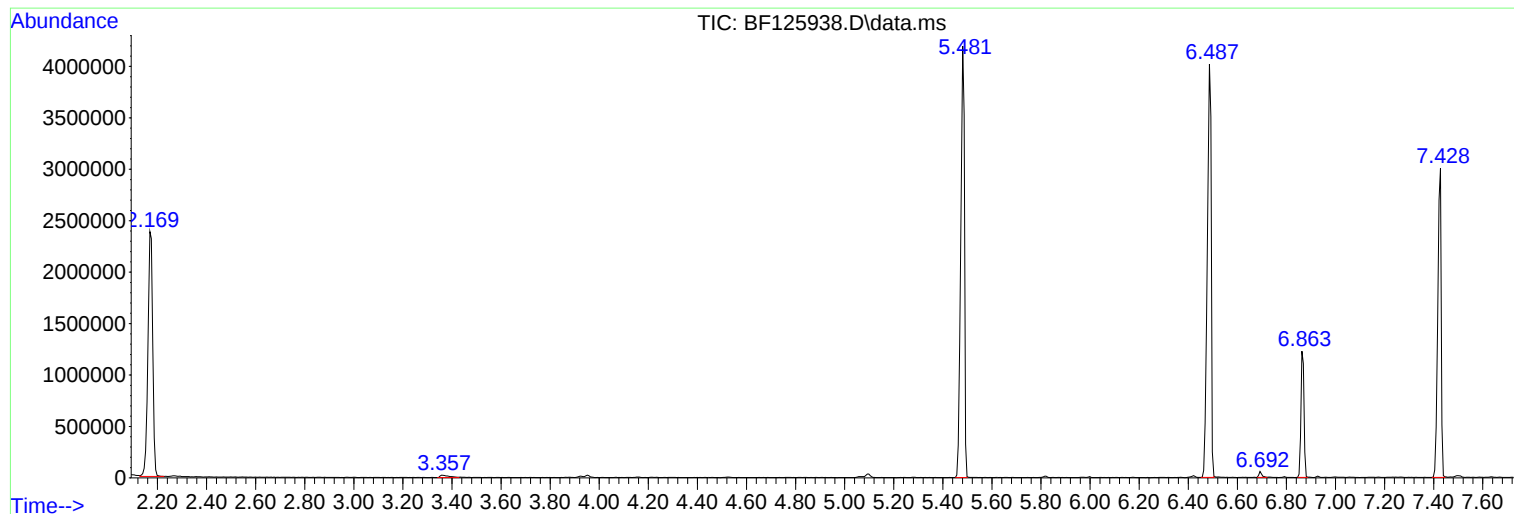
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF102521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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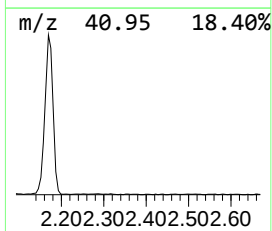
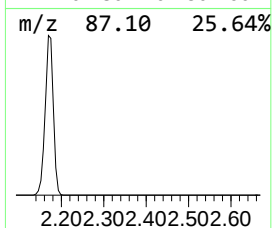
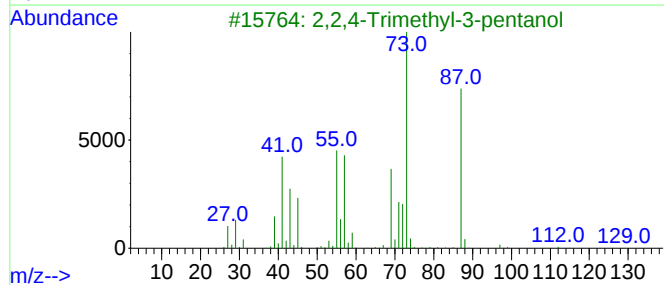
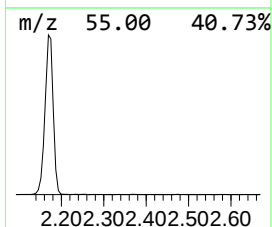
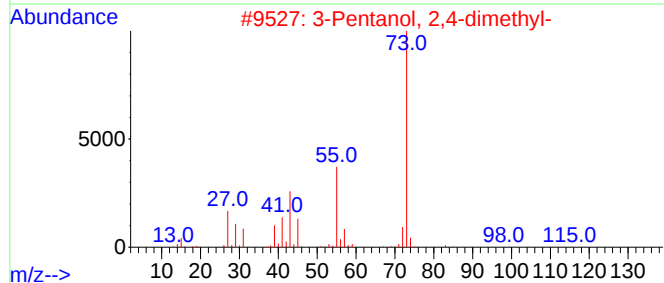
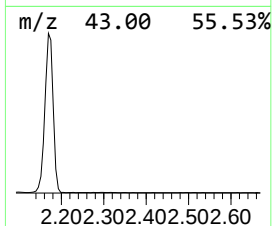
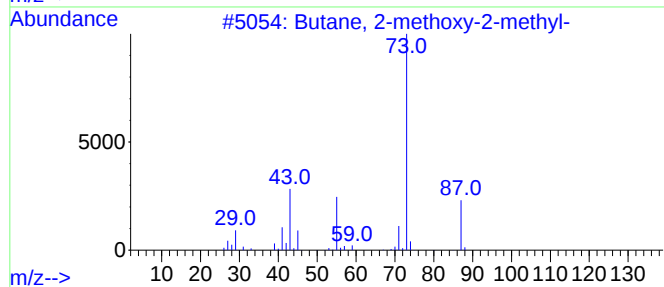
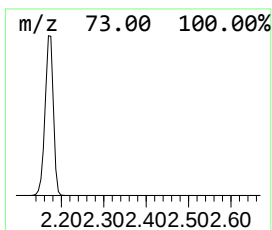
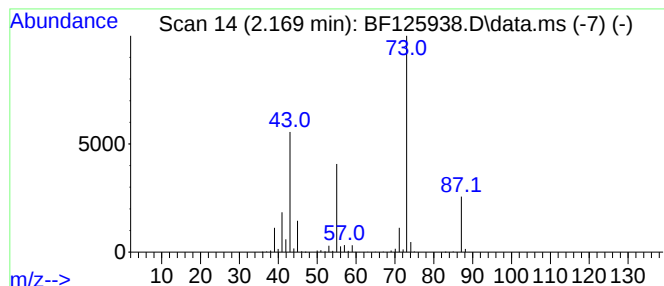
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.169	60.52 ng	3209110	1,4-Dichlorobenzene-d4	6.863

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			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
5			3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	25



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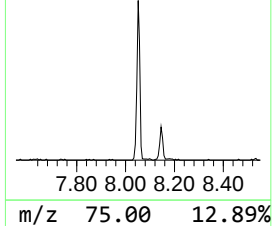
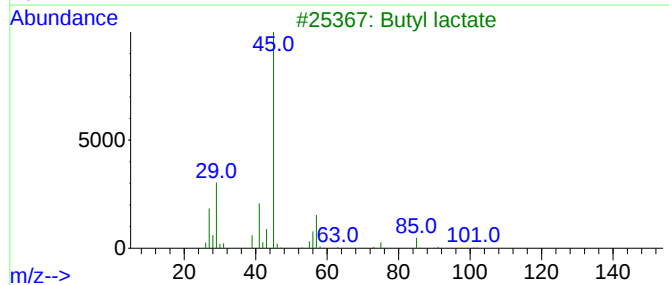
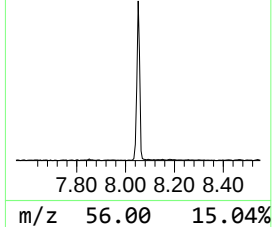
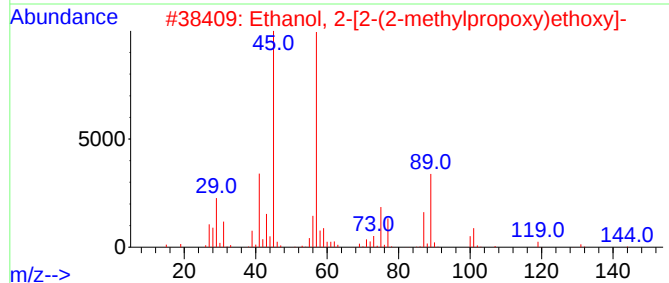
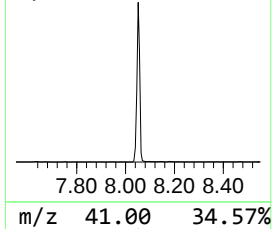
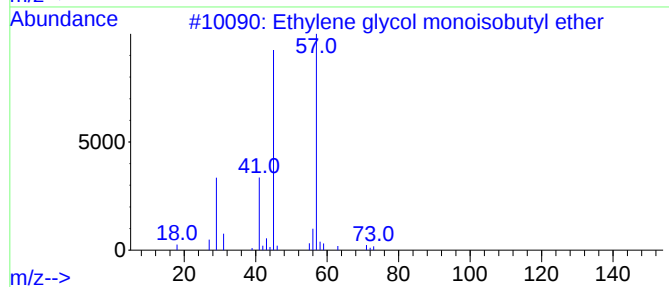
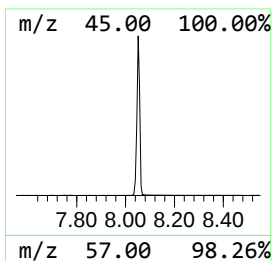
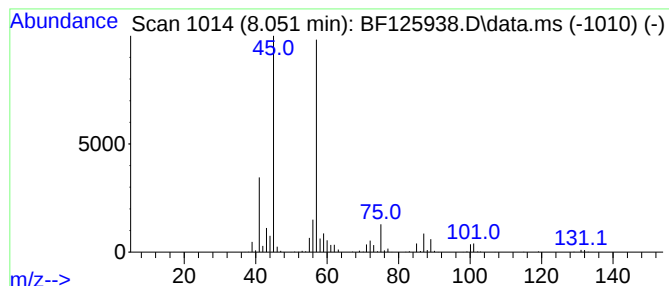
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Peak Number 2 Ethylene glycol monoisobuty... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	19.01 ng	1307970	Naphthalene-d8	8.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
3			Butyl lactate	146	C7H14O3	000138-22-7	50
4			1-Methoxy-3-methyl-3-butene	100	C6H12O	034752-58-4	47
5			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	47



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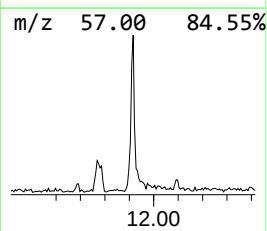
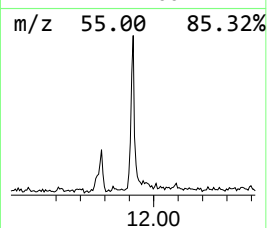
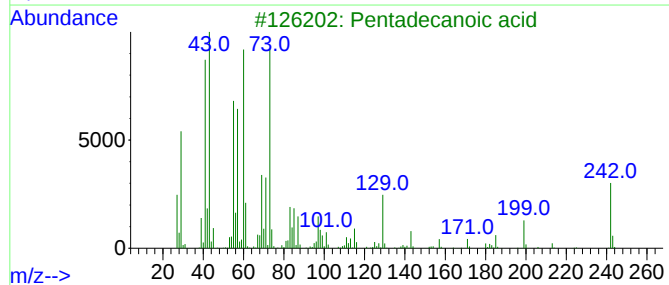
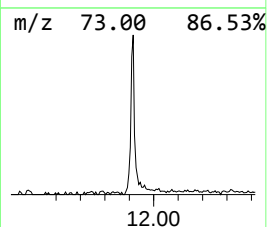
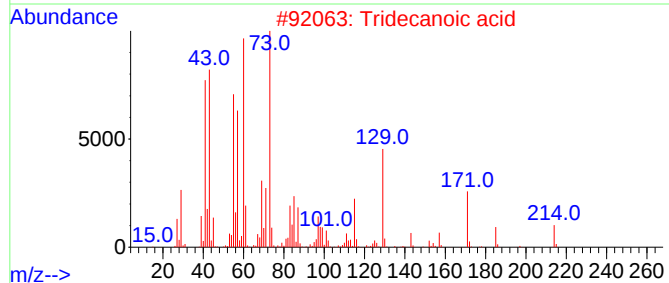
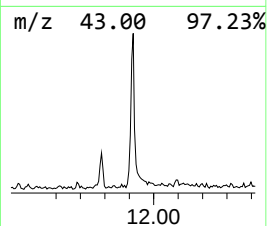
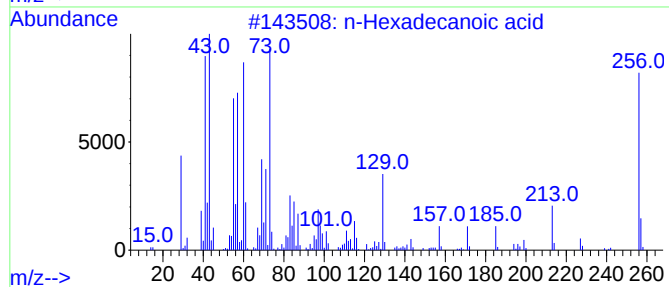
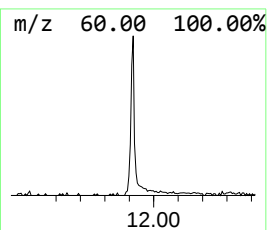
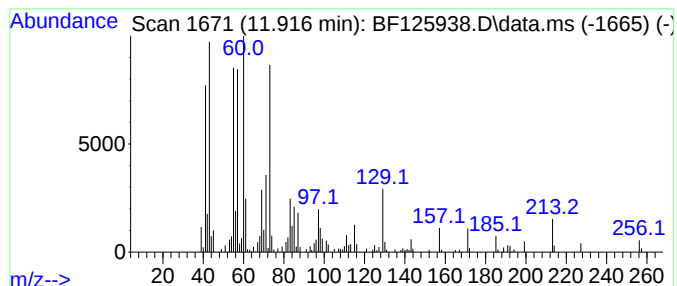
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.916	4.79 ng	373173	Phenanthrene-d10	11.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Octanoic acid	144	C8H16O2	000124-07-2	53



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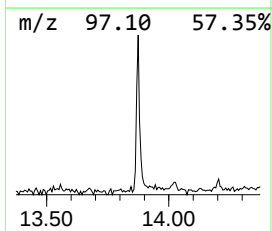
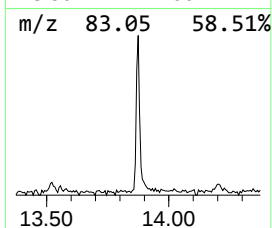
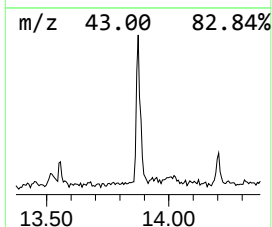
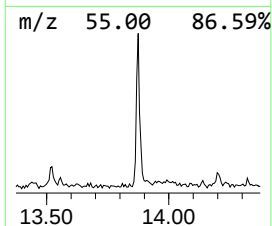
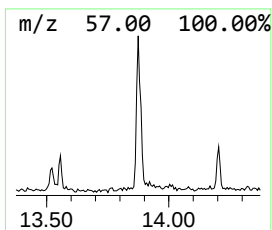
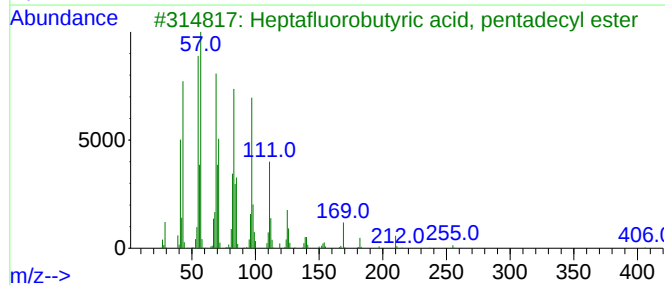
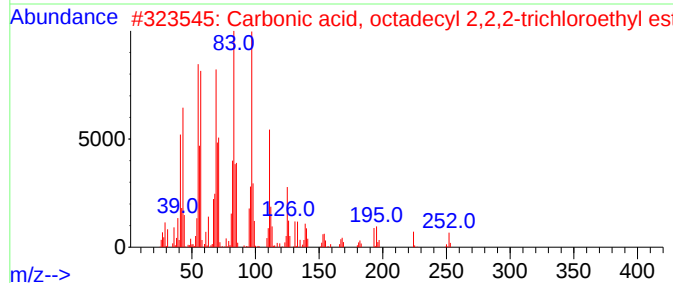
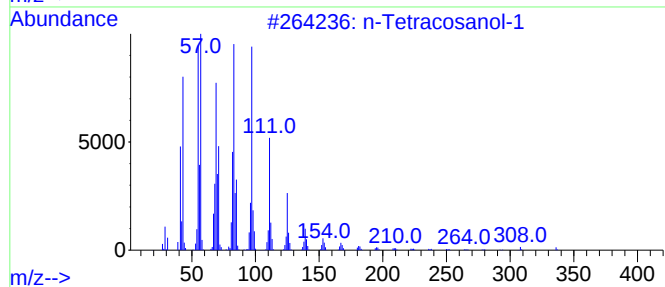
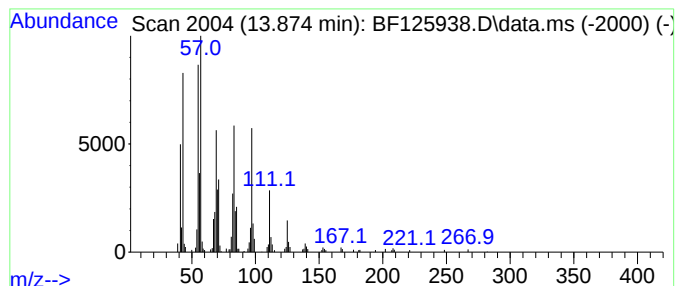
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Peak Number 4 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.874	6.25 ng	319561	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	91		
2	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	91		
3	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91		
4	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91		
5	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91		



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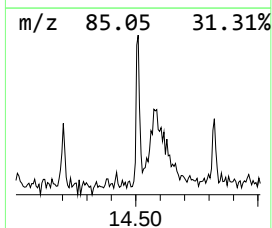
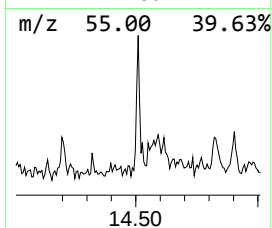
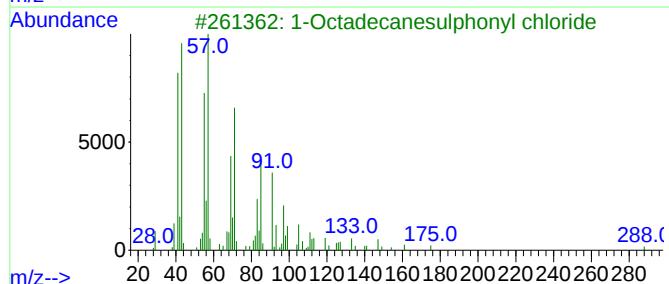
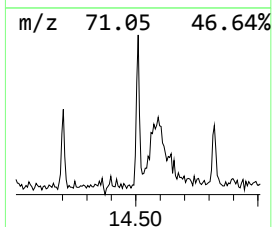
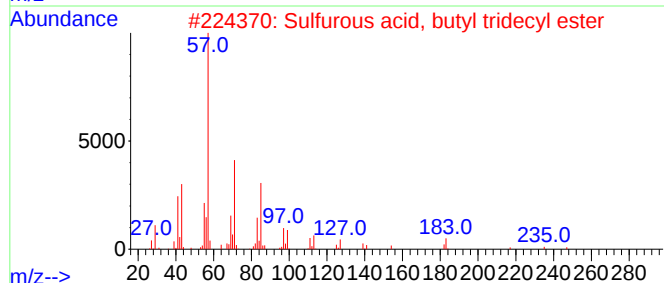
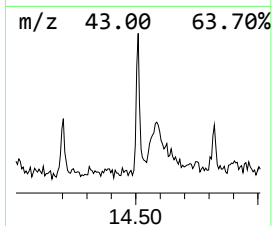
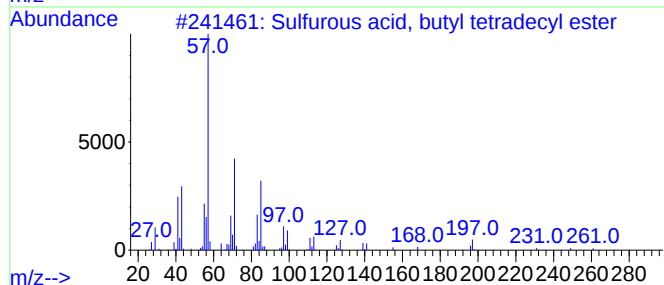
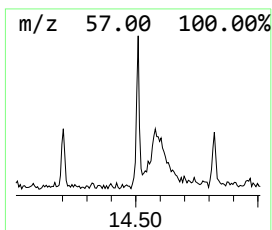
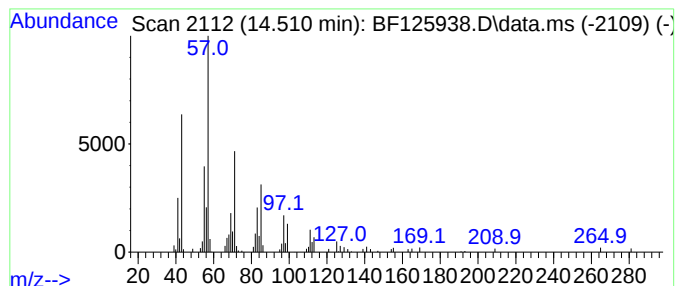
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Sulfurous acid, butyl tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.510	2.01 ng	102581	Chrysene-d12	14.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	90
2			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	90
3			1-Octadecanesulphonyl chloride	352	C18H37ClO2S	1000342-70-4	87
4			Isobutyl octadecyl ether	326	C22H46O	1000406-32-9	86
5			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.169	60.5	ng	3209110	1	6.863	1060570	20.0
Ethylene glycol...	8.051	19.0	ng	1307970	2	8.145	1376350	20.0
n-Hexadecanoic ...	11.916	4.8	ng	373173	4	11.386	1559740	20.0
n-Tetracosanol-1	13.874	6.3	ng	319561	5	14.021	1022080	20.0
Sulfurous acid,...	14.510	2.0	ng	102581	5	14.021	1022080	20.0