

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF081921\
 Data File : BF125123.D
 Acq On : 19 Aug 2021 19:58
 Operator : JU/CG
 Sample : M3430-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PE-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-BF081821.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125123.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	16	23	28	rVB	1370753	1807725	45.21%	5.785%
2	2.569	75	82	89	rVB3	23170	44486	1.11%	0.142%
3	5.145	512	520	526	rBV	102034	125179	3.13%	0.401%
4	5.534	581	586	589	rBV	3747819	3656155	91.45%	11.701%
5	5.763	621	625	629	rVB	54403	52137	1.30%	0.167%
6	6.539	751	757	760	rBV	3256082	3768115	94.25%	12.059%
7	6.916	818	821	825	rVB	1206478	992865	24.83%	3.177%
8	7.481	912	917	920	rBV	2726049	2437943	60.98%	7.802%
9	8.098	1018	1022	1025	rBV	1217742	932680	23.33%	2.985%
10	8.198	1036	1039	1043	rVB	1474317	1306786	32.69%	4.182%
11	9.274	1218	1222	1226	rBV	4204716	3998082	100.00%	12.795%
12	9.957	1334	1338	1341	rBV	1804000	1399101	34.99%	4.477%
13	10.745	1467	1472	1475	rBV	2734991	2525259	63.16%	8.081%
14	10.857	1487	1491	1496	rBV3	44041	62126	1.55%	0.199%
15	11.445	1587	1591	1593	rBV	1584596	1355862	33.91%	4.339%
16	11.463	1593	1594	1597	rVB	82385	57748	1.44%	0.185%
17	11.963	1670	1679	1687	rBV2	252880	296930	7.43%	0.950%
18	12.651	1794	1796	1800	rBV	140894	128383	3.21%	0.411%
19	12.745	1809	1812	1820	rBV	81311	99147	2.48%	0.317%
20	12.886	1831	1836	1841	rVB	114954	133568	3.34%	0.427%
21	13.027	1856	1860	1864	rBV	3450997	3362955	84.11%	10.762%
22	13.939	2010	2015	2031	rBV6	126095	397638	9.95%	1.273%
23	14.080	2035	2039	2042	rVV	1051009	1010672	25.28%	3.234%
24	14.104	2042	2043	2050	rVB	67953	63890	1.60%	0.204%
25	14.592	2122	2126	2134	rBV9	35648	81510	2.04%	0.261%
26	15.133	2215	2218	2222	rBV	59677	91081	2.28%	0.291%
27	15.445	2268	2271	2276	rVB3	48357	59433	1.49%	0.190%
28	15.509	2279	2282	2285	rVB	41315	40811	1.02%	0.131%
29	15.580	2289	2294	2298	rBV	728989	913989	22.86%	2.925%
30	17.074	2545	2548	2553	rBV7	28011	45192	1.13%	0.145%

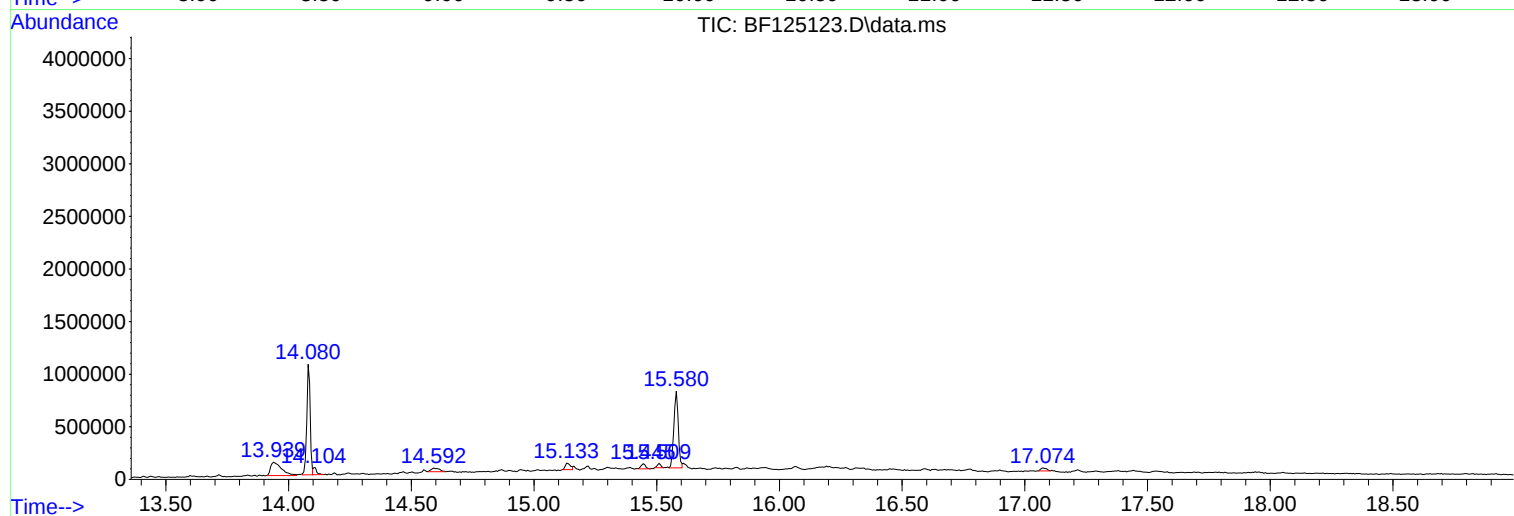
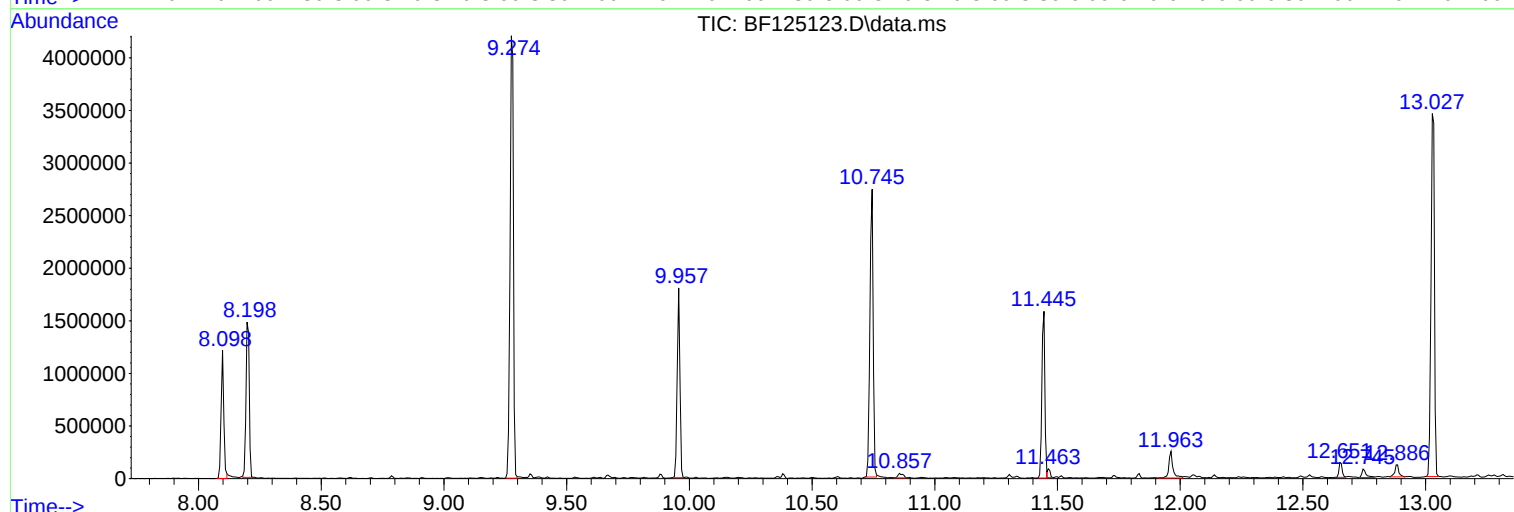
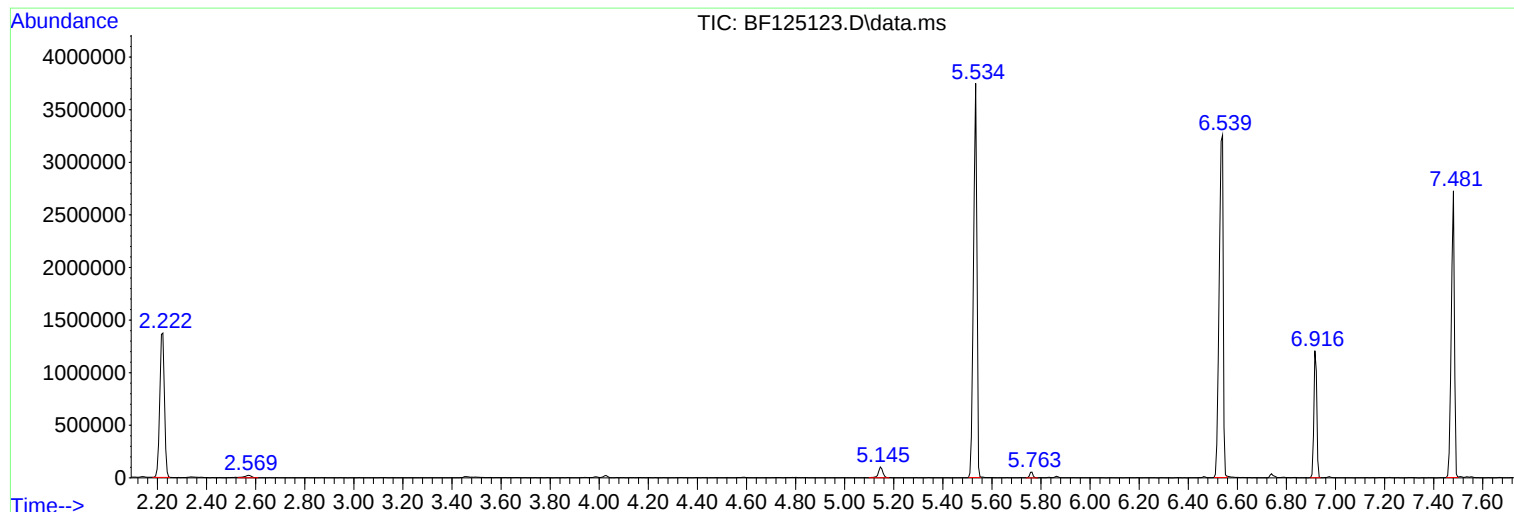
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ClientSampleId :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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ClientSampled :
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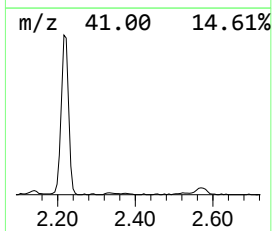
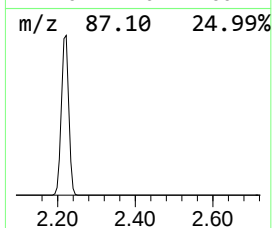
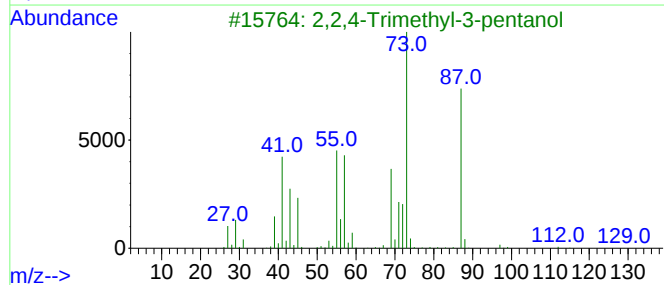
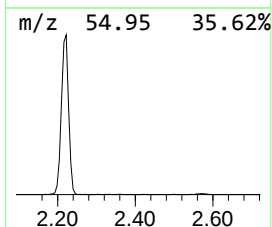
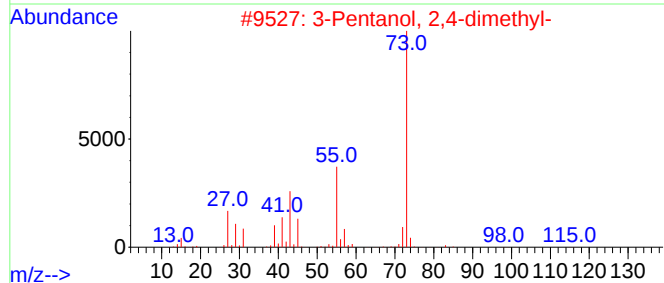
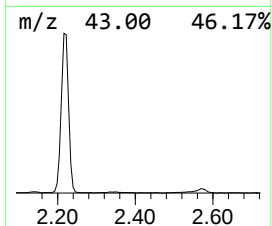
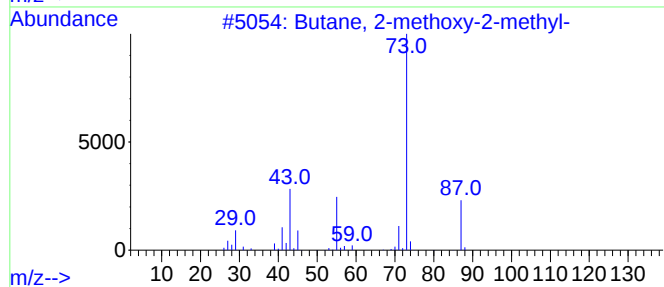
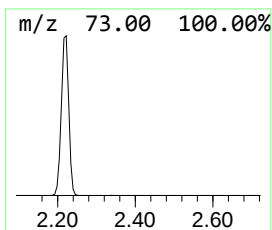
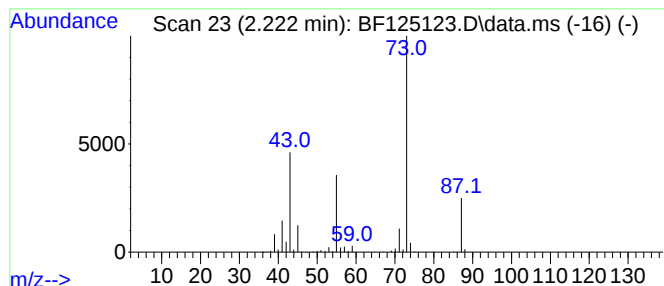
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.222	36.41 ng	1807730	1,4-Dichlorobenzene-d4	6.916

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			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28



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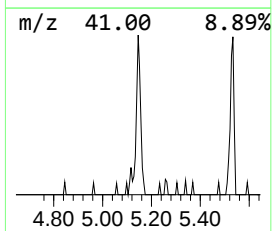
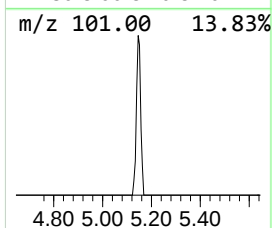
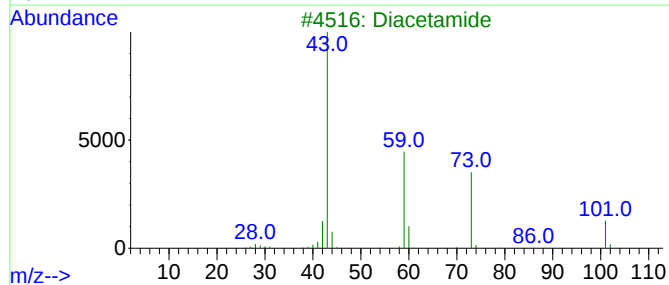
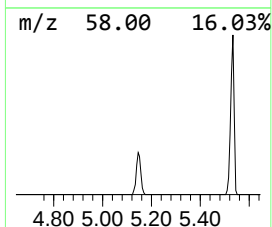
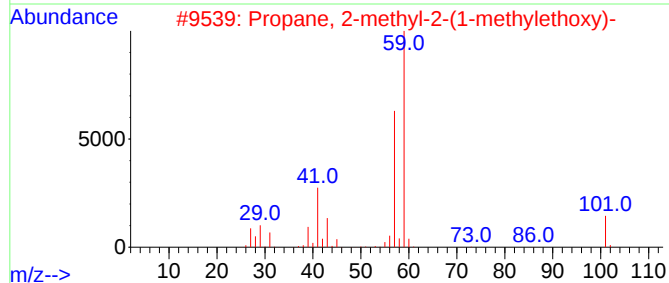
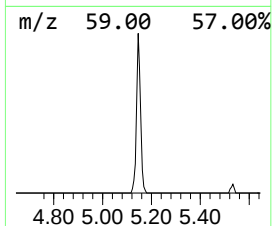
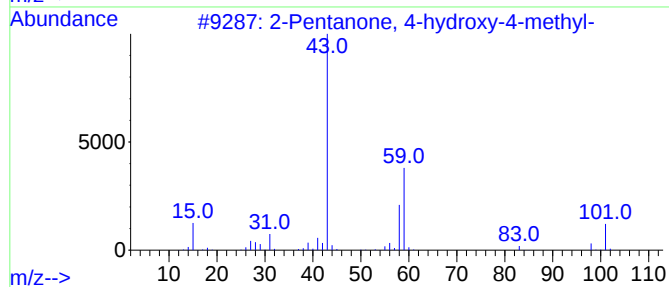
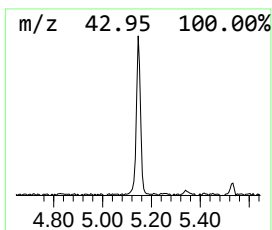
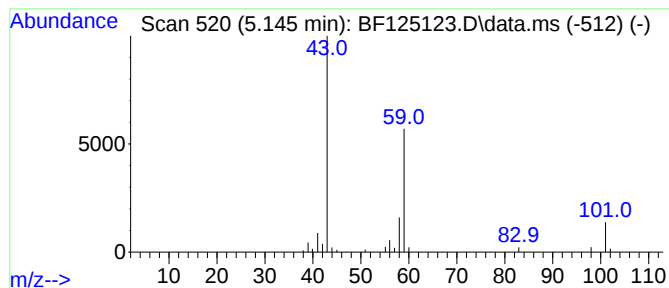
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.145	2.52 ng	125179	1,4-Dichlorobenzene-d4	6.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36		
3	Diacetamide	101	C4H7NO2	000625-77-4	36		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28		



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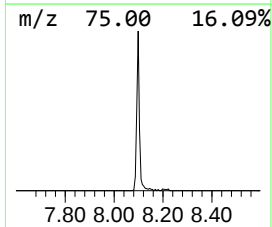
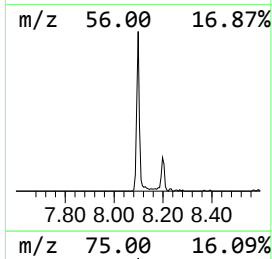
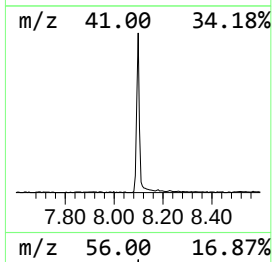
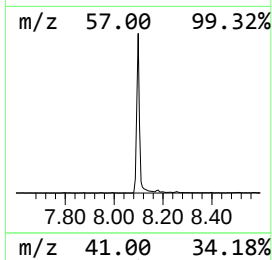
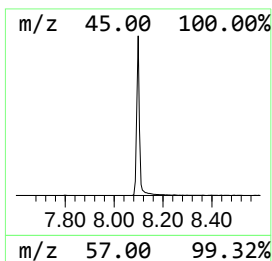
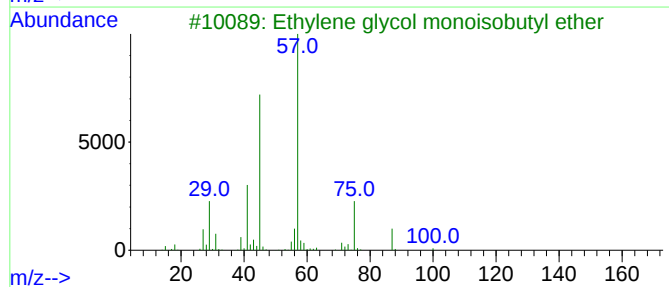
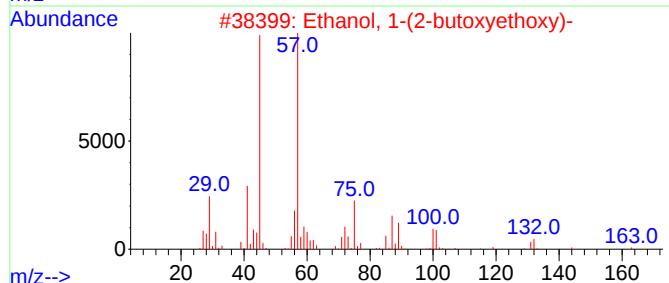
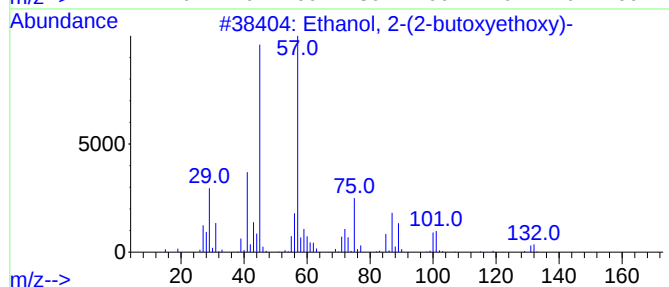
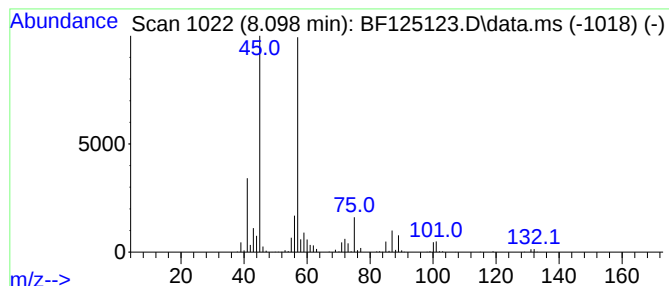
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.098	14.27 ng	932680	Naphthalene-d8	8.198

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	59
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Butyl lactate	146	C7H14O3	000138-22-7	47



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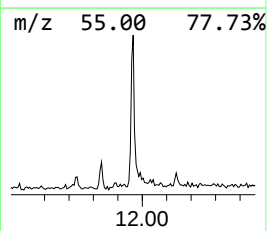
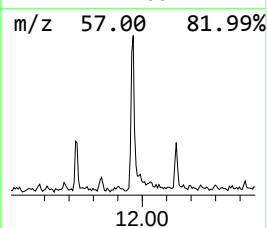
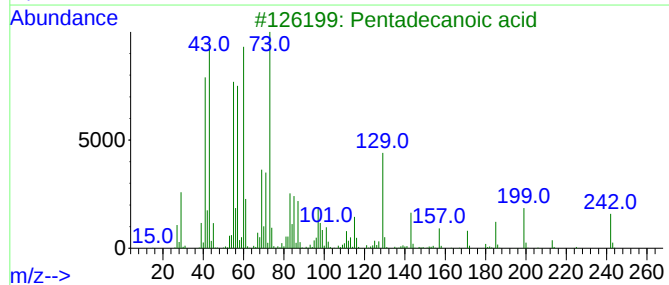
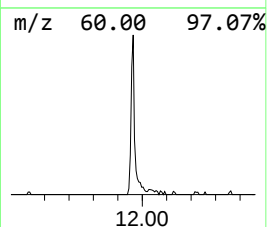
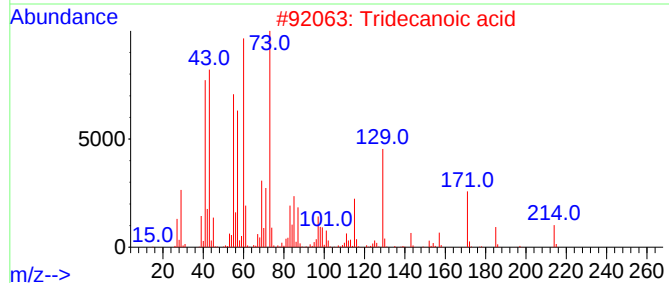
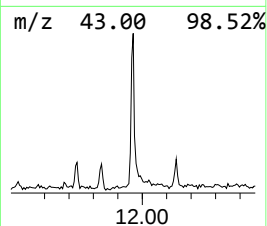
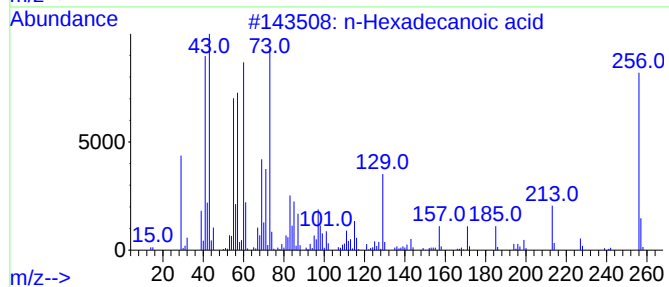
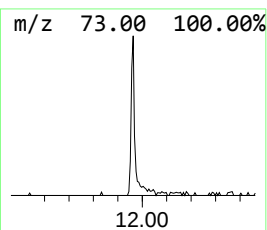
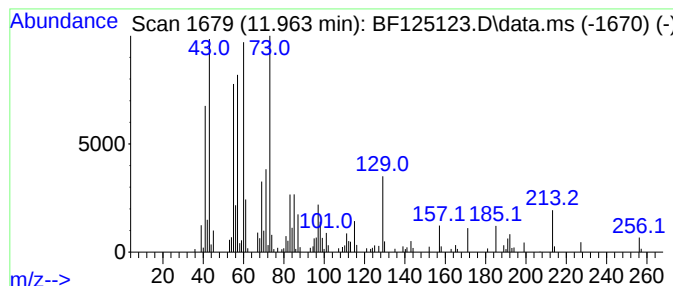
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.963	4.38 ng	296930	Phenanthrene-d10	11.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Nonanoic acid	158	C9H18O2	000112-05-0	50



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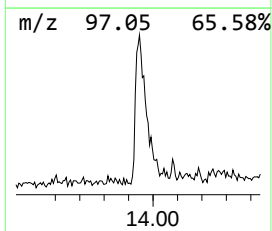
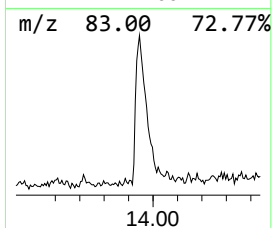
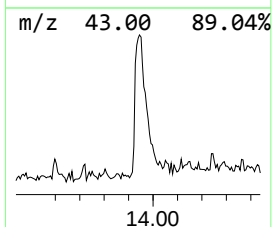
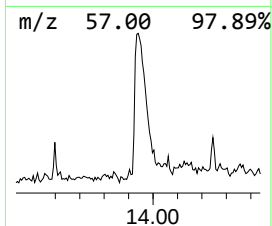
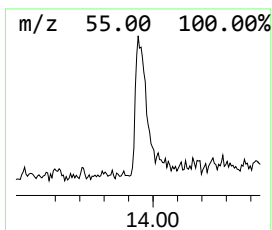
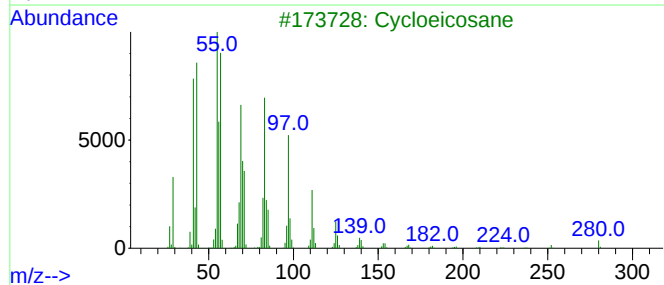
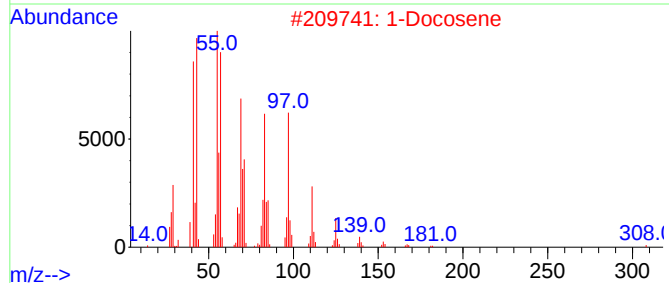
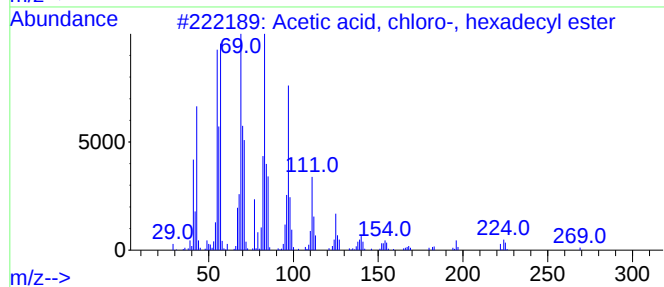
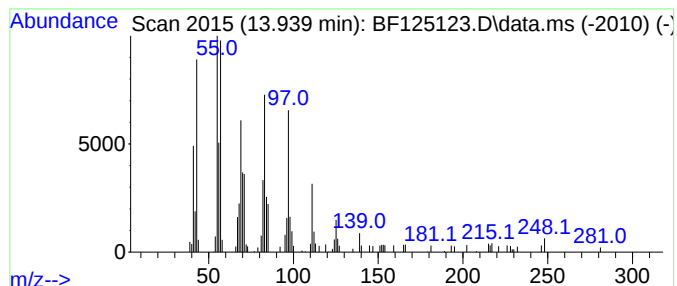
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Peak Number 6 Acetic acid, chloro-, hexad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.939	7.87 ng	397638	Chrysene-d12	14.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	95
2			1-Docosene	308	C22H44	001599-67-3	94
3			Cycloeicosane	280	C20H40	000296-56-0	90
4			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	90
5			1-Octadecene	252	C18H36	000112-88-9	90



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.222	36.4	ng	1807730	1	6.916	992865	20.0
2-Pentanone, 4-...	5.145	2.5	ng	125179	1	6.916	992865	20.0
Ethanol, 2-(2-b...	8.098	14.3	ng	932680	2	8.198	1306790	20.0
n-Hexadecanoic ...	11.963	4.4	ng	296930	4	11.445	1355860	20.0
Acetic acid, ch...	13.939	7.9	ng	397638	5	14.080	1010670	20.0