

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091321\
 Data File : BF125449.D
 Acq On : 13 Sep 2021 18:01
 Operator : JU/CG
 Sample : M3684-08
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A019145

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: BF125449.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	12	19	25	rBV	1175347	1479127	42.46%	5.712%
2	2.310	33	38	43	rVB	48188	64892	1.86%	0.251%
3	5.110	510	514	526	rVB	142726	172676	4.96%	0.667%
4	5.516	578	583	586	rBV	2883073	2872984	82.48%	11.096%
5	6.522	749	754	757	rBV	2967220	2858118	82.05%	11.038%
6	6.881	812	815	819	rBV	999038	907591	26.06%	3.505%
7	6.945	823	826	833	rBV2	24105	39052	1.12%	0.151%
8	7.451	906	912	922	rBV	1815293	1897100	54.46%	7.327%
9	8.075	1014	1018	1030	rBV	114669	293438	8.42%	1.133%
10	8.169	1030	1034	1047	rVB	1371437	1227591	35.24%	4.741%
11	9.245	1212	1217	1220	rBV	3754014	3274363	94.00%	12.646%
12	9.516	1259	1263	1270	rBV	63560	57430	1.65%	0.222%
13	9.928	1329	1333	1336	rBV	1557858	1332737	38.26%	5.147%
14	10.716	1463	1467	1478	rBV	2393120	2261275	64.92%	8.733%
15	11.416	1582	1586	1593	rBV	1591443	1376712	39.52%	5.317%
16	11.933	1669	1674	1683	rBV2	158049	186167	5.34%	0.719%
17	12.722	1804	1808	1816	rBV	40761	55125	1.58%	0.213%
18	13.004	1852	1856	1859	rBV	3984256	3483293	100.00%	13.453%
19	13.957	2010	2018	2030	rBV5	65820	248173	7.12%	0.958%
20	14.063	2032	2036	2047	rVB	1141041	1032428	29.64%	3.987%
21	15.557	2285	2290	2298	rBV	608415	772867	22.19%	2.985%

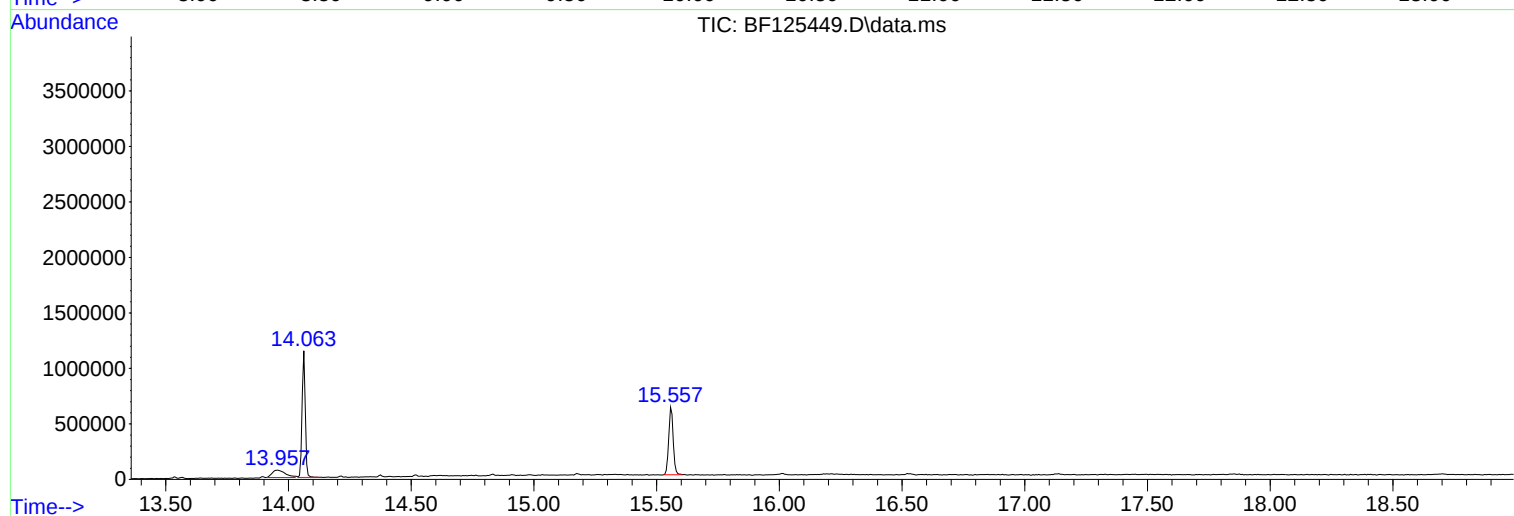
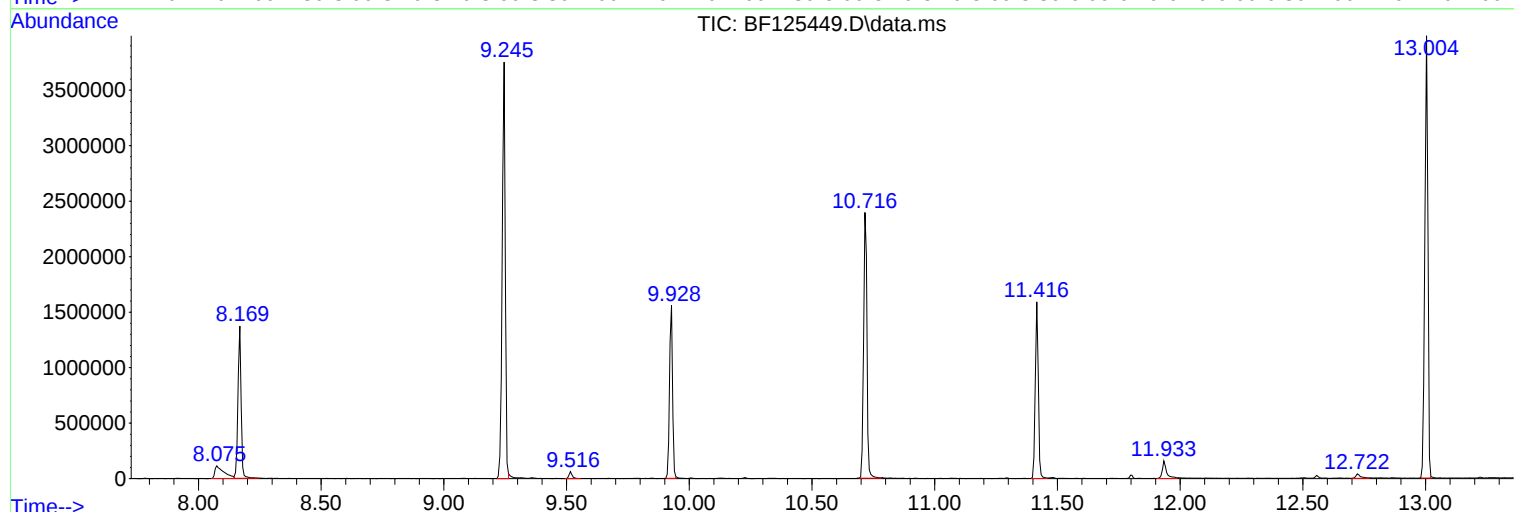
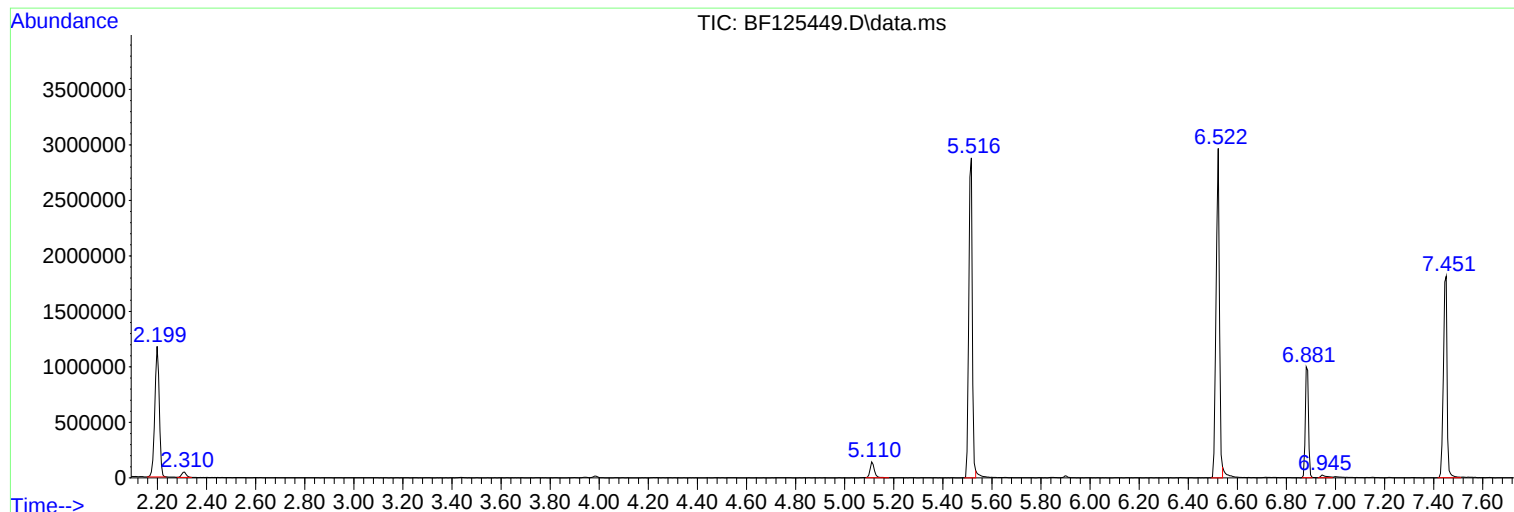
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF081821.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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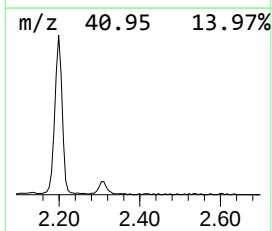
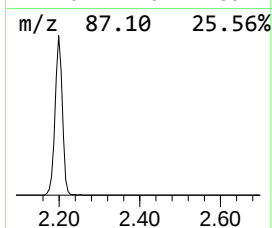
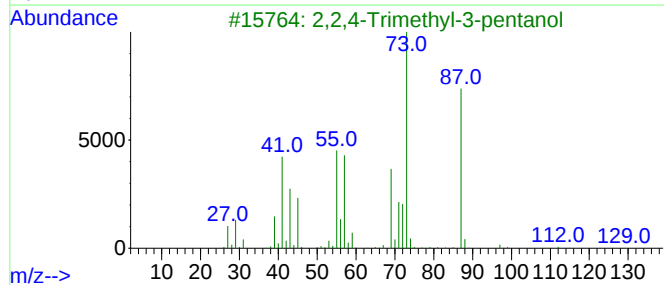
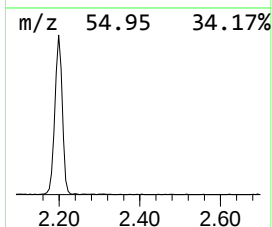
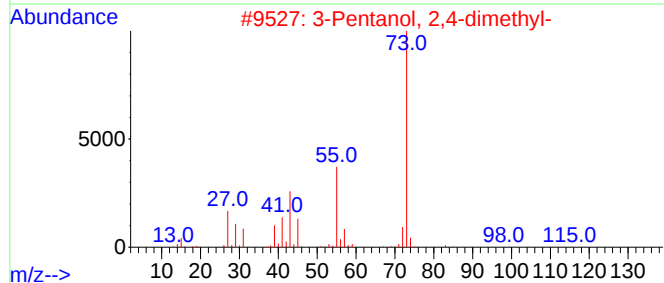
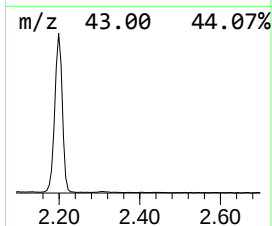
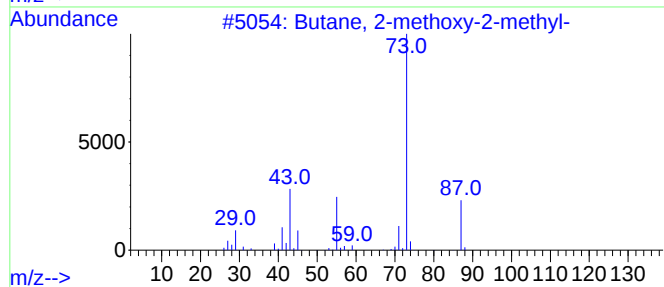
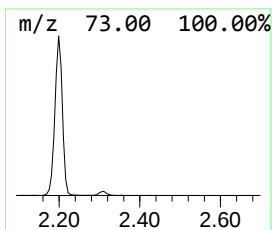
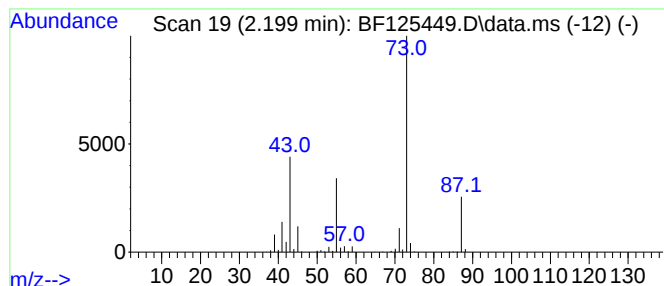
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.199	32.59 ng	1479130	1,4-Dichlorobenzene-d4	6.887

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	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	32
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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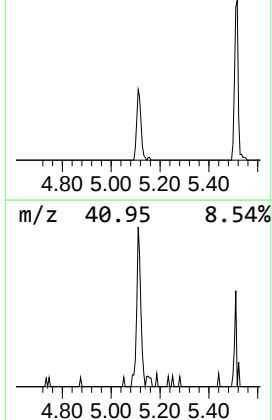
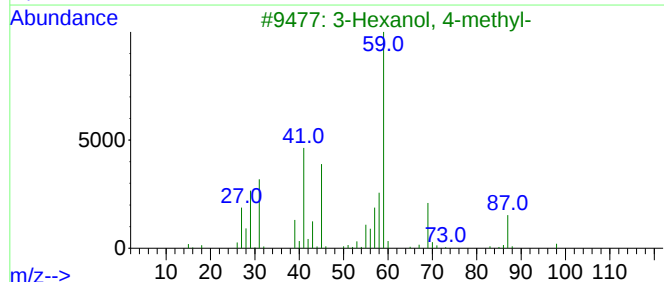
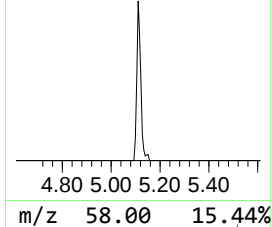
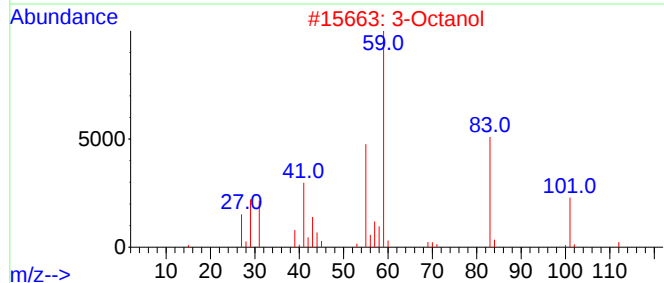
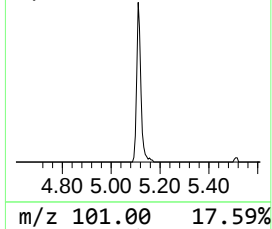
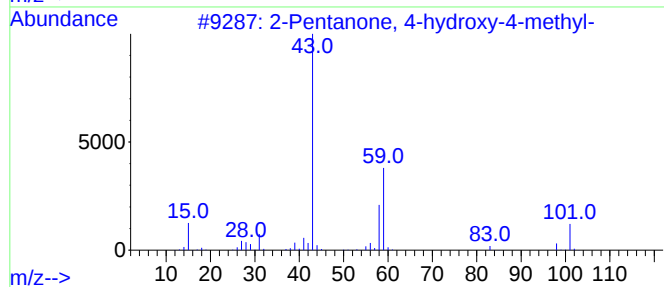
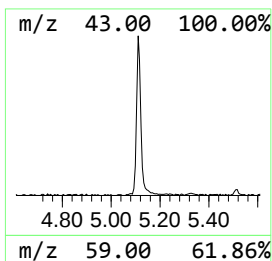
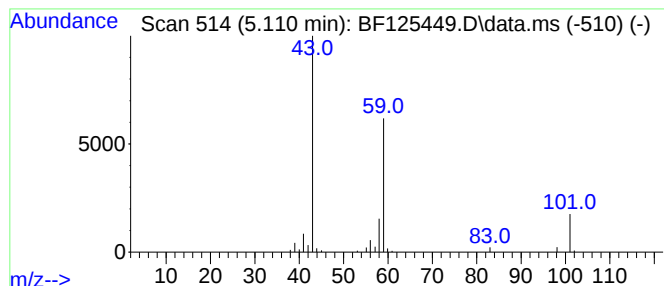
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.110	3.81 ng	172676	1,4-Dichlorobenzene-d4	6.887

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		3-Octanol	130	C8H18O	000589-98-0	33
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	9



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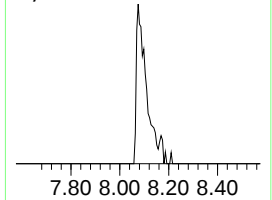
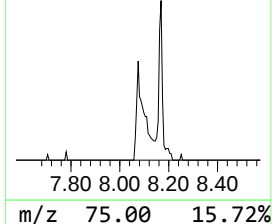
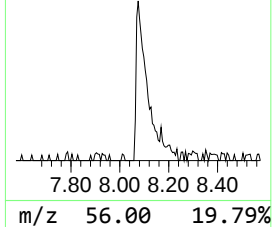
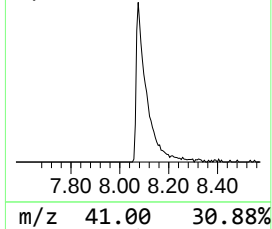
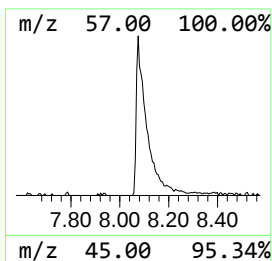
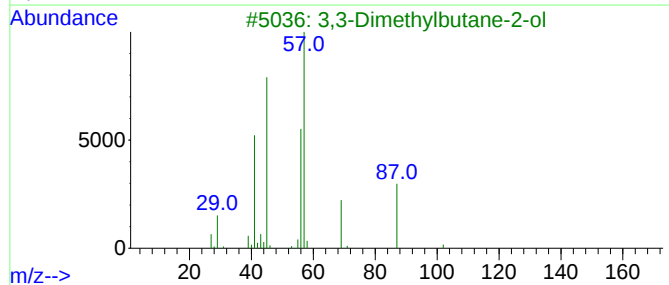
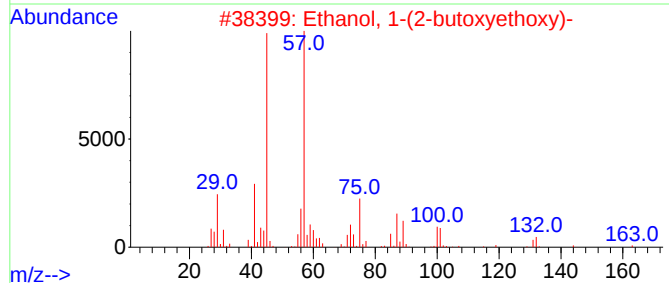
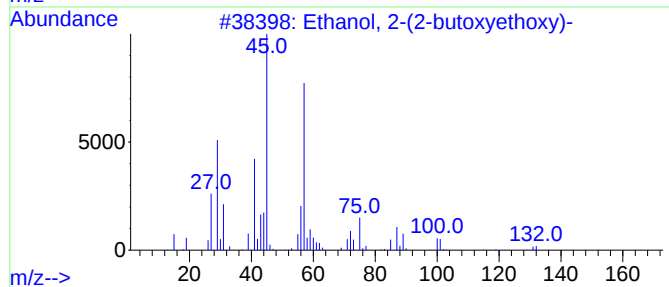
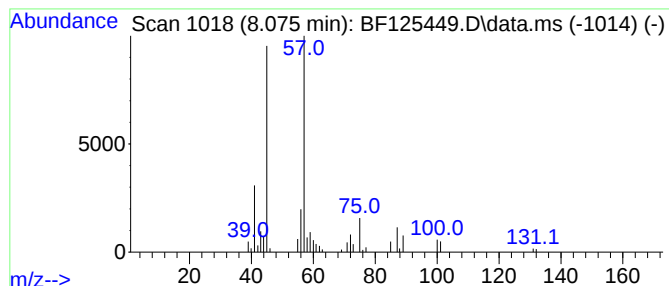
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.075	4.78 ng	293438	Naphthalene-d8	8.169

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	83
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	72
3			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	45



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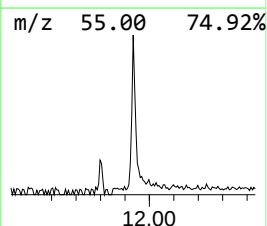
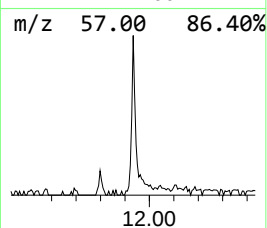
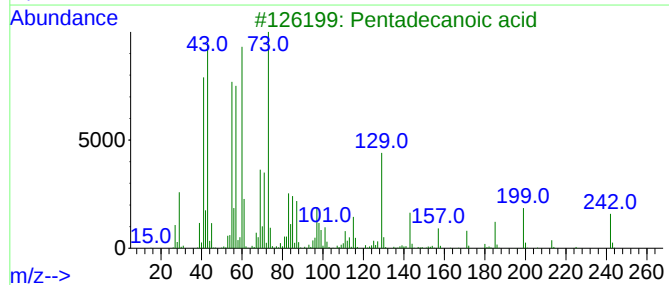
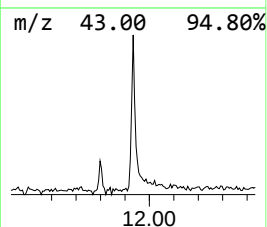
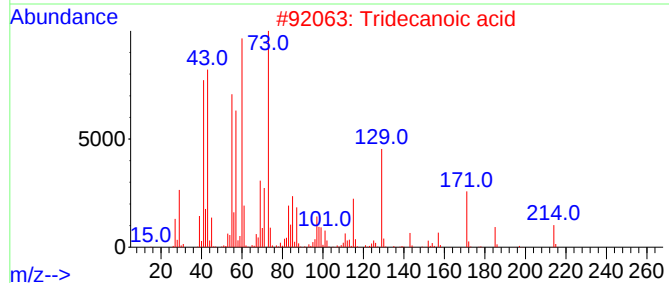
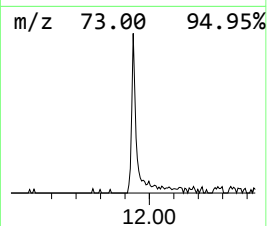
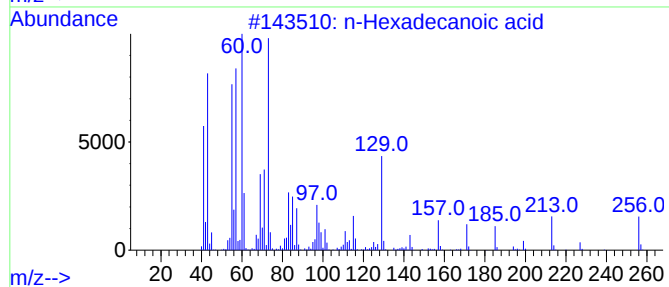
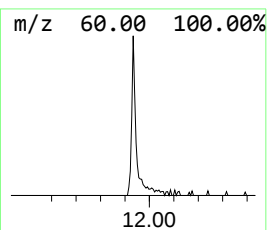
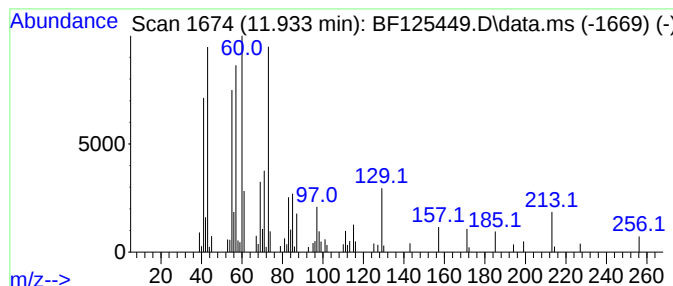
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	2.70 ng	186167	Phenanthrene-d10	11.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	78
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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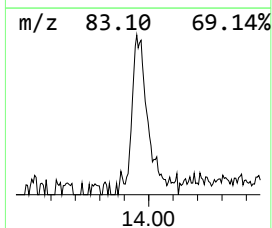
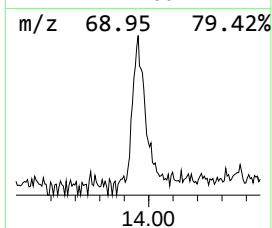
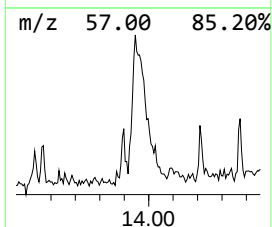
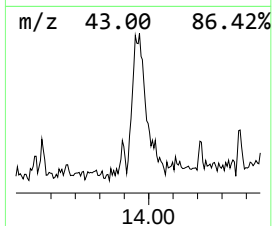
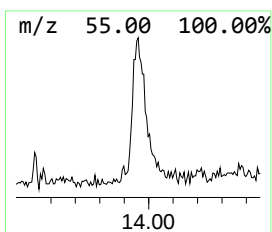
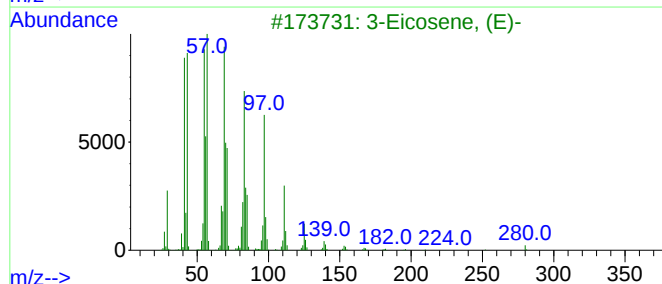
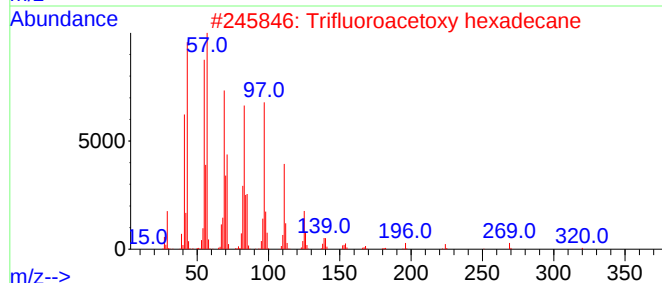
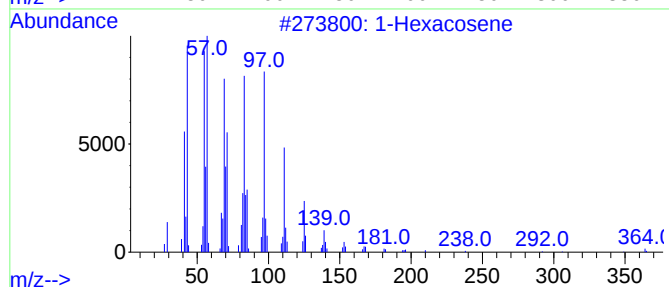
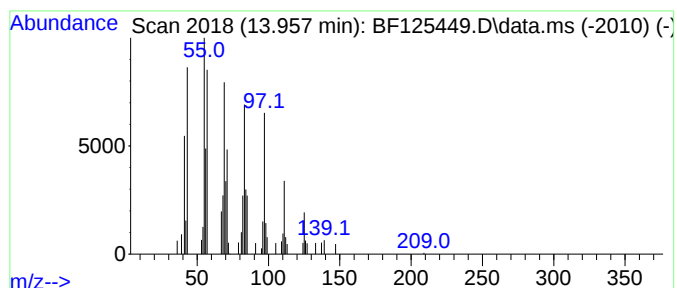
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexacosene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.957	4.81 ng	248173	Chrysene-d12	14.063

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexacosene			364	C26H52	018835-33-1	91
2	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	90
3	3-Eicosene, (E)-			280	C20H40	074685-33-9	90
4	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	90
5	1-Hexacosanol			382	C26H54O	000506-52-5	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.199	32.6	ng	1479130	1	6.887	907591	20.0
2-Pentanone, 4-...	5.110	3.8	ng	172676	1	6.887	907591	20.0
Ethanol, 2-(2-b...	8.075	4.8	ng	293438	2	8.169	1227590	20.0
n-Hexadecanoic ...	11.933	2.7	ng	186167	4	11.416	1376710	20.0
1-Hexacosene	13.957	4.8	ng	248173	5	14.063	1032430	20.0