

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM102221\
 Data File : BM032672.D
 Acq On : 22 Oct 2021 13:07
 Operator : CG/JU
 Sample : M4294-07
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 WC-2-GS

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_M\Methods\8270-BM100221.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM032672.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.637	301	306	316	rBV	170522	247153	3.35%	0.519%
2	5.131	384	390	408	rBV	3563347	5218693	70.70%	10.950%
3	6.754	658	666	680	rBV	3507864	5473946	74.15%	11.485%
4	7.542	794	800	809	rBV	932493	1417504	19.20%	2.974%
5	8.701	988	997	1010	rBV	2305788	3676585	49.80%	7.714%
6	10.113	1230	1237	1248	rBV	689253	1074519	14.56%	2.254%
7	10.330	1266	1274	1287	rBV	1198391	1971659	26.71%	4.137%
8	12.818	1690	1697	1712	rBV	5003791	7381978	100.00%	15.488%
9	14.201	1923	1932	1943	rBV	1609801	2372970	32.15%	4.979%
10	15.695	2180	2186	2205	rBV	3215490	4584840	62.11%	9.620%
11	16.936	2391	2397	2403	rBV	1659380	2328791	31.55%	4.886%
12	17.612	2508	2512	2516	rVB	101283	114929	1.56%	0.241%
13	17.836	2546	2550	2557	rBV	138194	198001	2.68%	0.415%
14	18.995	2743	2747	2751	rBV	84442	123736	1.68%	0.260%
15	19.359	2806	2809	2816	rVB	62145	83427	1.13%	0.175%
16	19.565	2838	2844	2849	rBV	5100331	6328359	85.73%	13.278%
17	20.824	3055	3058	3063	rBV	413740	432355	5.86%	0.907%
18	21.118	3103	3108	3112	rBV	1488528	1904237	25.80%	3.995%
19	21.636	3192	3196	3202	rBV	556419	804970	10.90%	1.689%
20	23.253	3466	3471	3481	rVB2	1165259	1922429	26.04%	4.034%

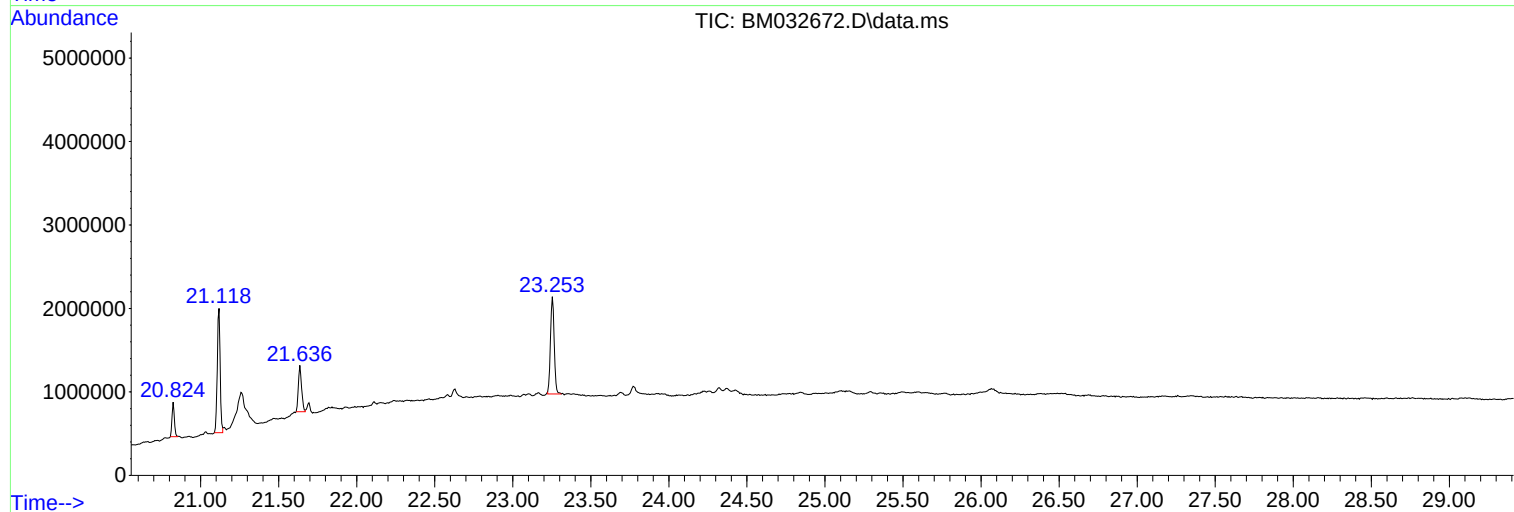
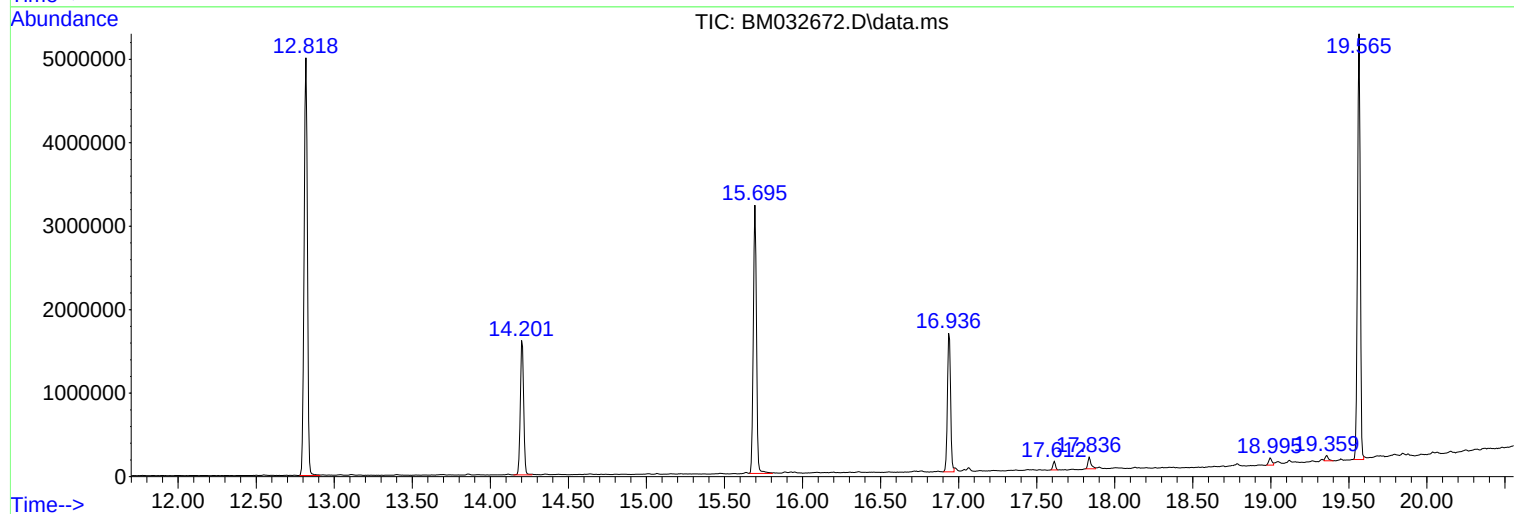
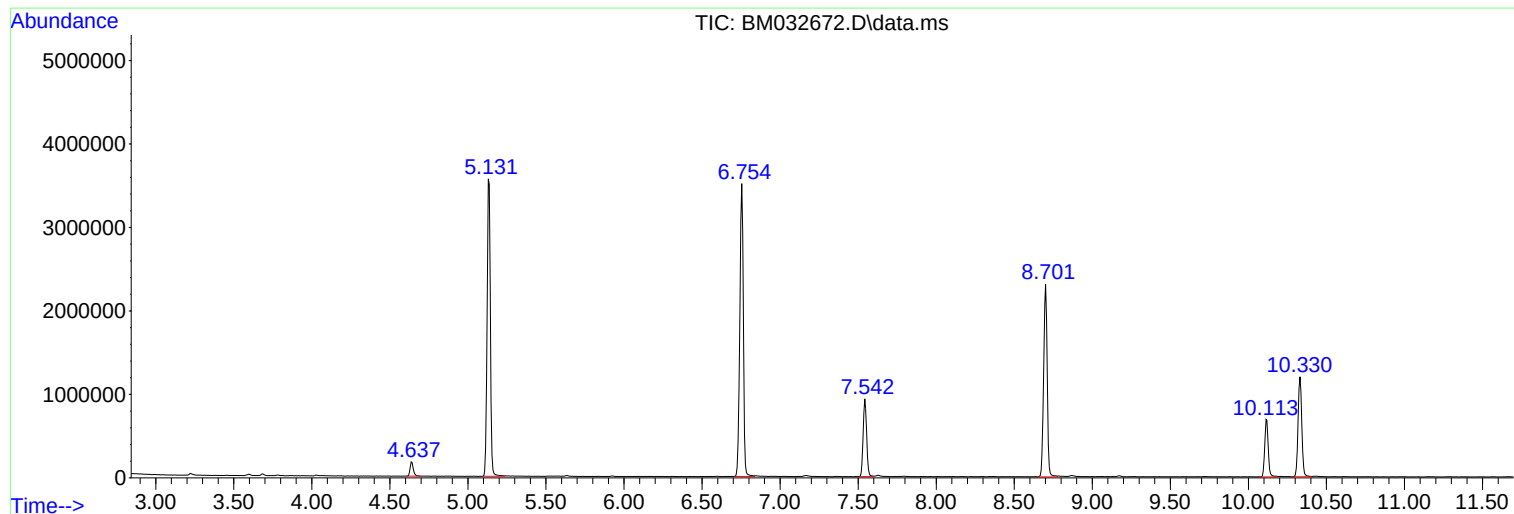
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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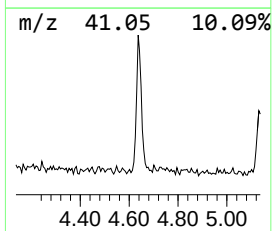
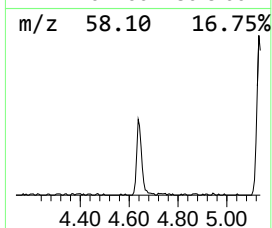
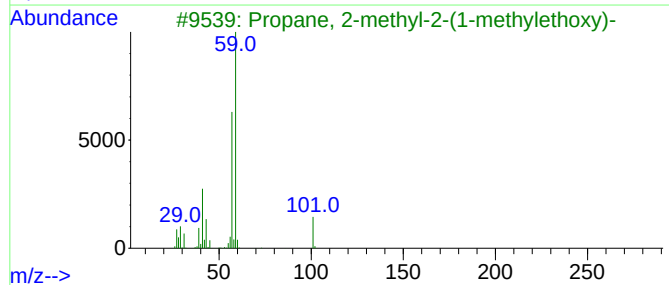
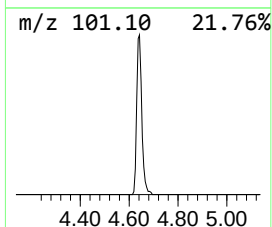
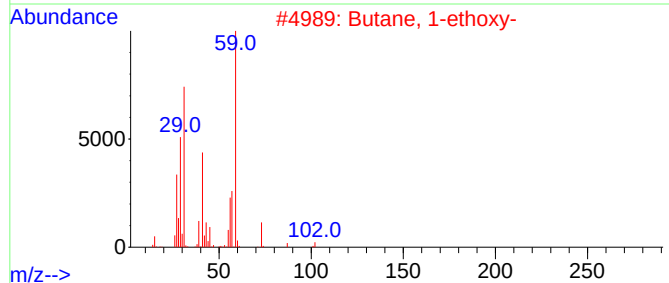
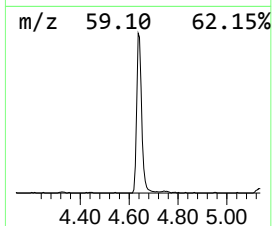
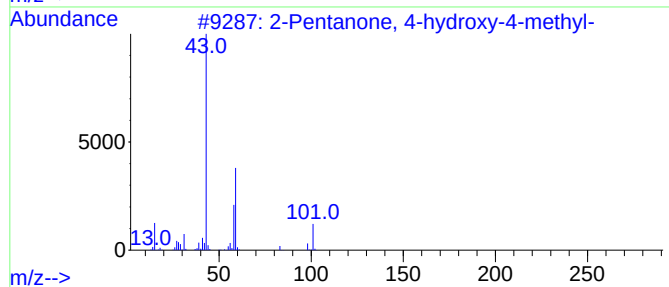
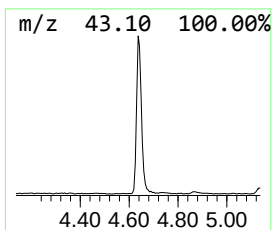
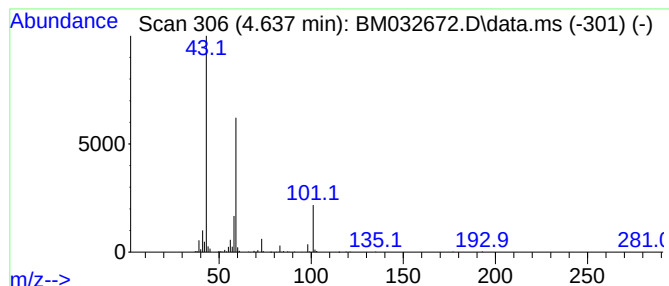
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM100221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.637	3.49 ng	247153	1,4-Dichlorobenzene-d4	7.542

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25		
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	25		
4	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	23		
5	Methyl 2,5,8,11-tetraoxatridecan...	236	C10H20O6	1000366-78-2	23		



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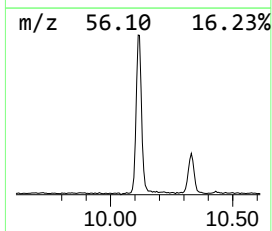
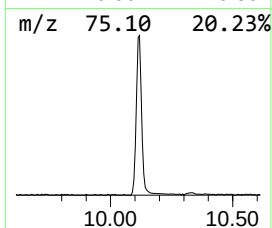
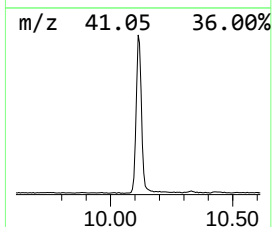
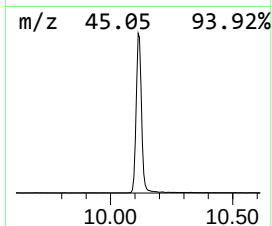
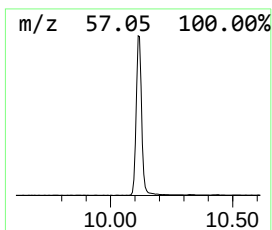
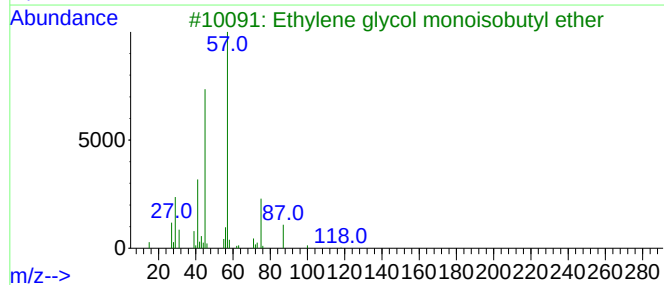
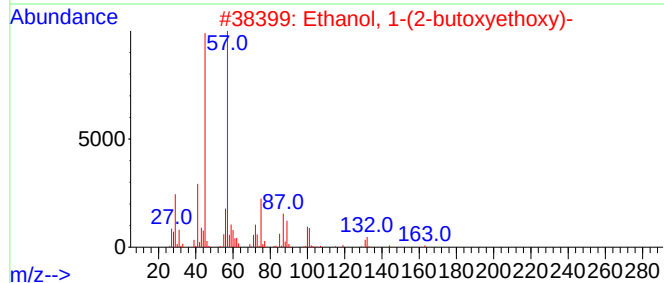
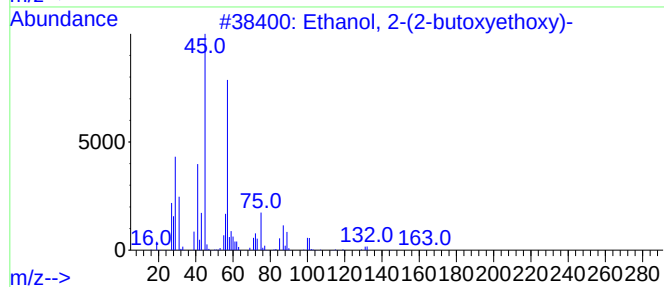
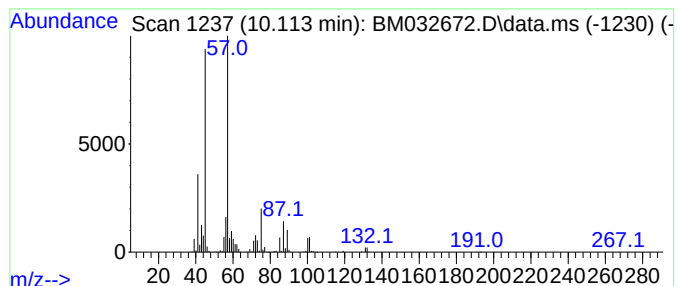
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.113	10.90 ng	1074520	Naphthalene-d8	10.330

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	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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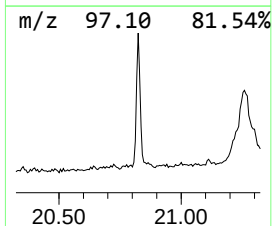
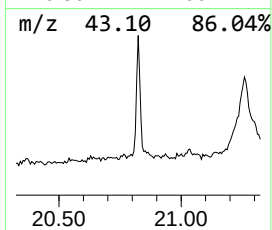
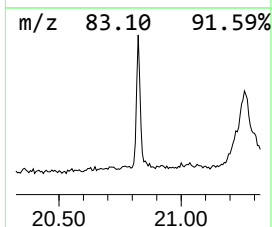
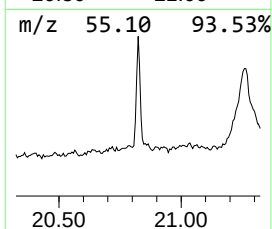
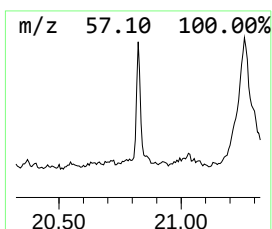
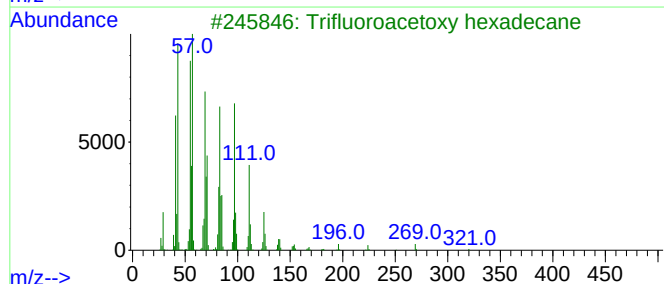
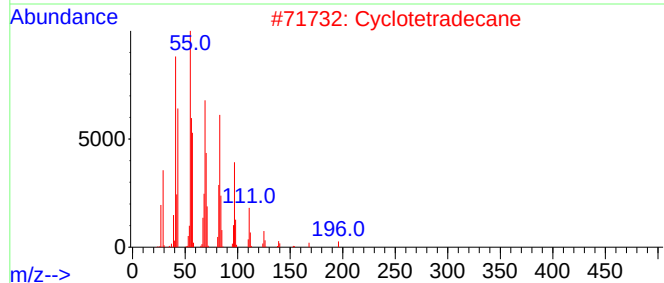
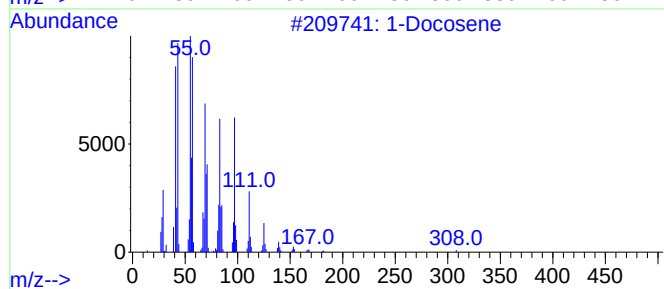
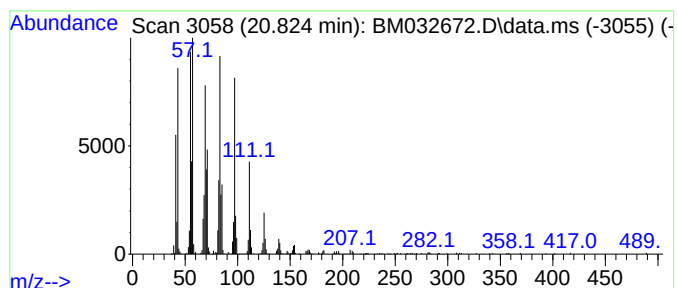
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Docosene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.824	4.54 ng	432355	Chrysene-d12	21.118

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	98
2	Cyclotetradecane			196	C14H28	000295-17-0	95
3	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
4	1-Heneicosanol			312	C21H44O	015594-90-8	94
5	Pentacos-1-ene			350	C25H50	016980-85-1	94



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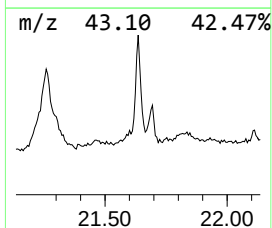
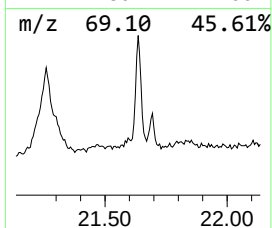
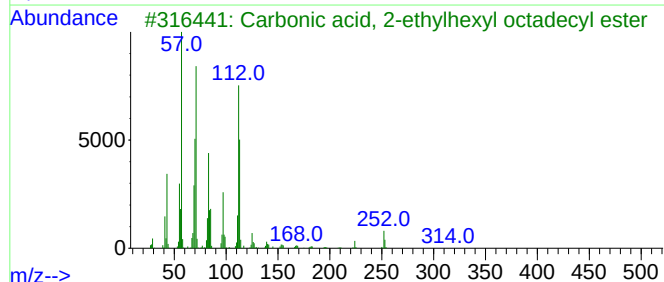
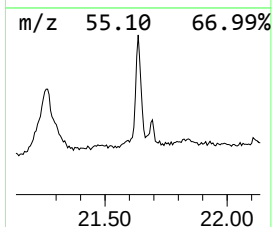
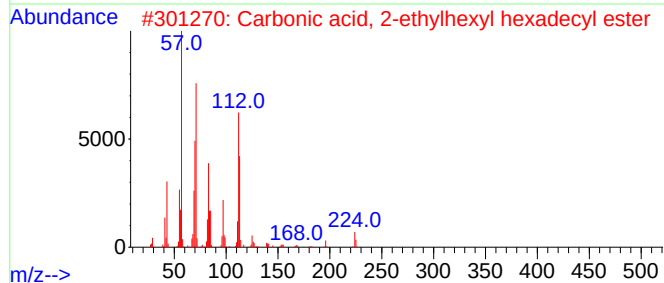
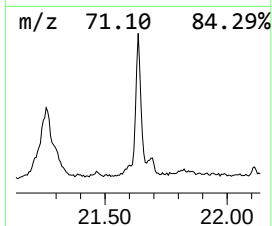
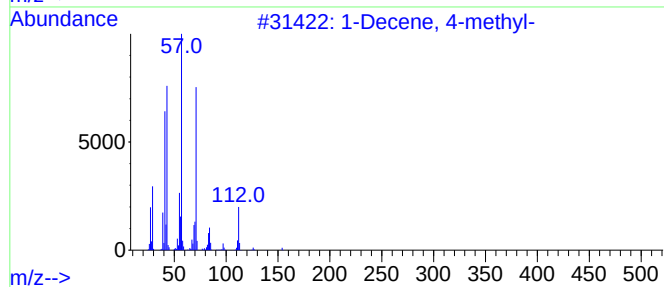
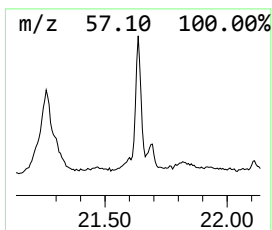
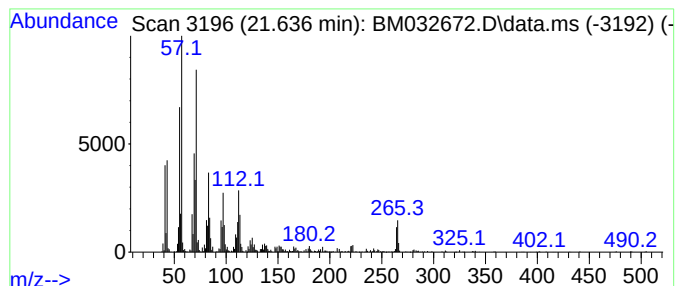
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown21.636 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.636	8.45 ng	804970	Chrysene-d12	21.118

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decene, 4-methyl-			154	C11H22	013151-29-6	49
2	Carbonic acid, 2-ethylhexyl hexa...			398	C25H50O3	1000383-14-3	49
3	Carbonic acid, 2-ethylhexyl octa...			426	C27H54O3	1000383-14-5	49
4	Heptane, 3-ethyl-5-methyl-			142	C10H22	052896-90-9	46
5	3-Eicosene, (E)-			280	C20H40	074685-33-9	41



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.637	3.5	ng	247153	1	7.542	1417500	20.0
Ethanol, 2-(2-b...	10.113	10.9	ng	1074520	2	10.330	1971660	20.0
1-Docosene	20.824	4.5	ng	432355	5	21.118	1904240	20.0
unknown21.636	21.636	8.4	ng	804970	5	21.118	1904240	20.0