

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110223\
 Data File : BF136110.D
 Acq On : 02 Nov 2023 22:37
 Operator : CG\JU
 Sample : 05050-08
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B3

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-BF103023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136110.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.063	502	506	514	rVB	80802	107416	3.03%	0.512%
2	5.451	566	572	575	rBV	2842807	3029190	85.43%	14.442%
3	6.457	736	743	746	rBV	2633185	3013521	84.98%	14.367%
4	6.645	772	775	789	rVB	62813	60848	1.72%	0.290%
5	6.816	801	804	808	rBV	745804	594474	16.76%	2.834%
6	7.381	895	900	903	rBV	1967313	2016306	56.86%	9.613%
7	8.098	1018	1022	1025	rBV	1071284	789409	22.26%	3.764%
8	9.180	1202	1206	1209	rBV	4349928	3545946	100.00%	16.905%
9	9.298	1223	1226	1230	rVB	52172	44668	1.26%	0.213%
10	9.857	1317	1321	1324	rBV	1128384	853555	24.07%	4.069%
11	10.651	1451	1456	1459	rBV	2227262	2031519	57.29%	9.685%
12	11.345	1571	1574	1578	rBV	874246	761469	21.47%	3.630%
13	11.886	1662	1666	1680	rBV2	218135	226322	6.38%	1.079%
14	12.680	1797	1801	1813	rBV	56240	71288	2.01%	0.340%
15	12.951	1842	1847	1850	rBV	3115105	2767808	78.06%	13.196%
16	13.898	2004	2008	2022	rVB5	23622	64746	1.83%	0.309%
17	14.004	2022	2026	2032	rVB	632399	544388	15.35%	2.595%
18	15.492	2273	2279	2287	rBV	380184	452236	12.75%	2.156%

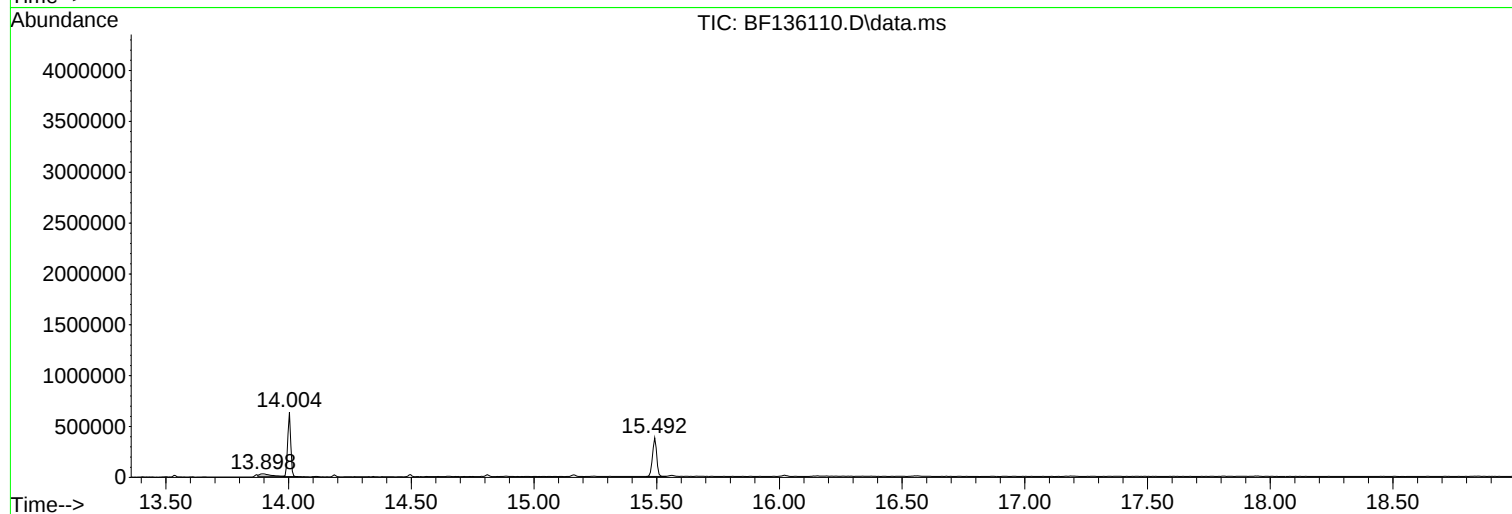
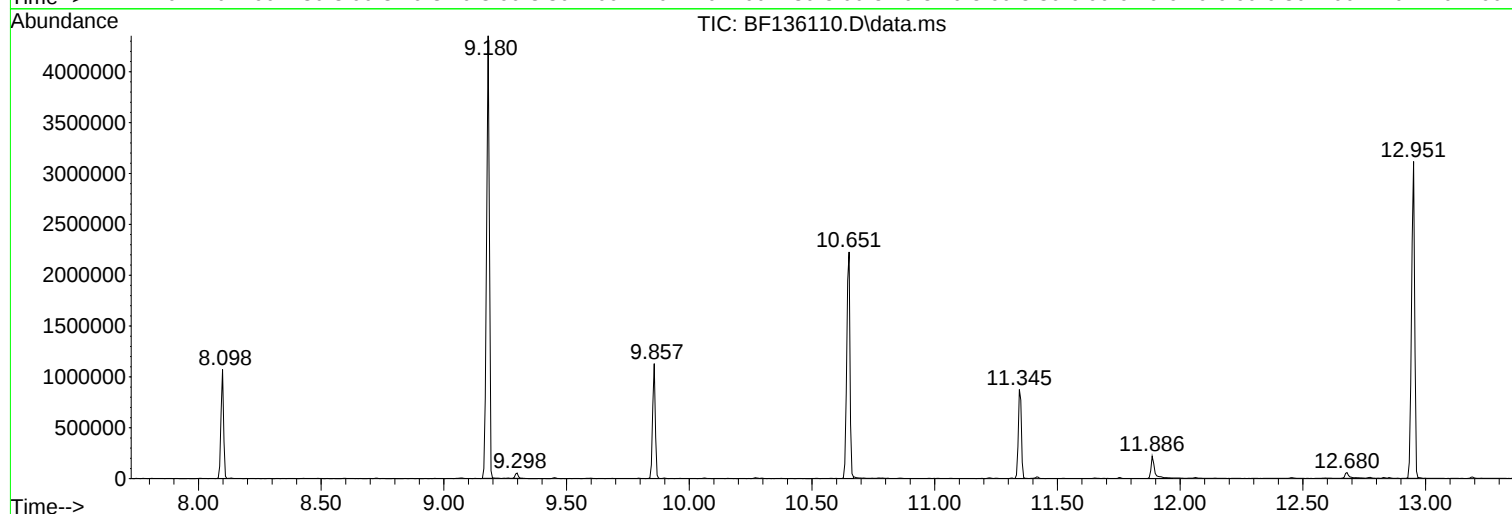
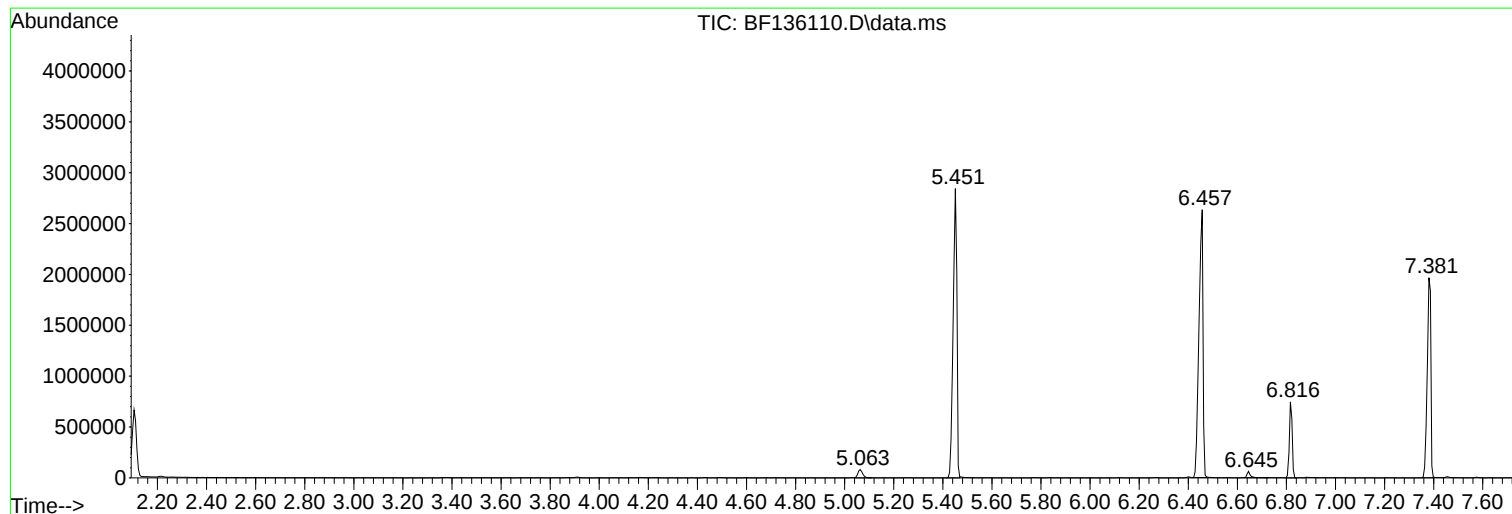
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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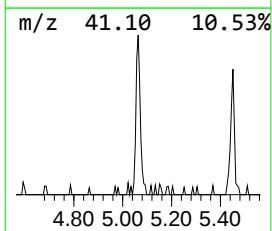
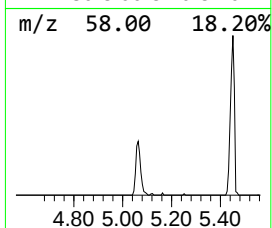
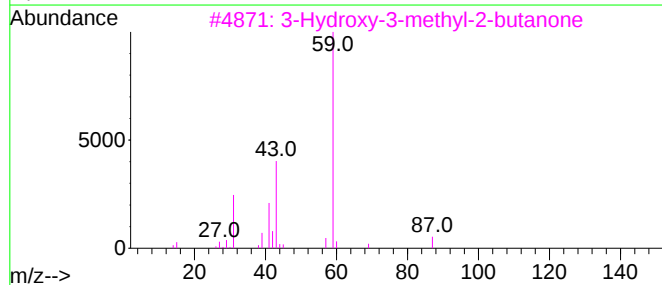
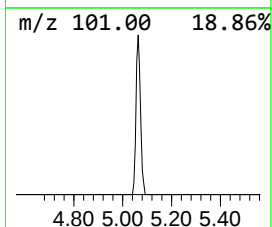
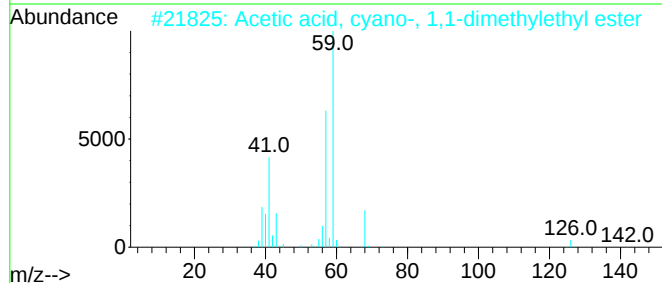
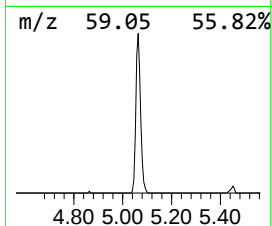
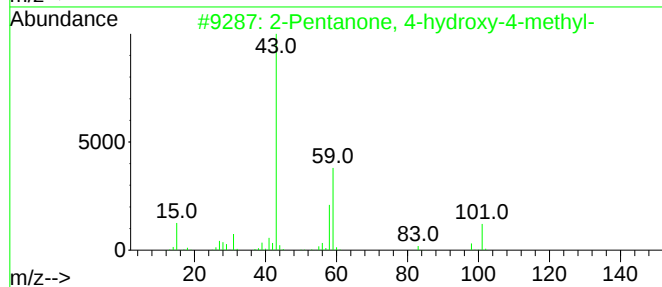
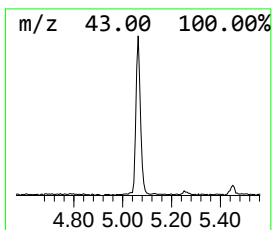
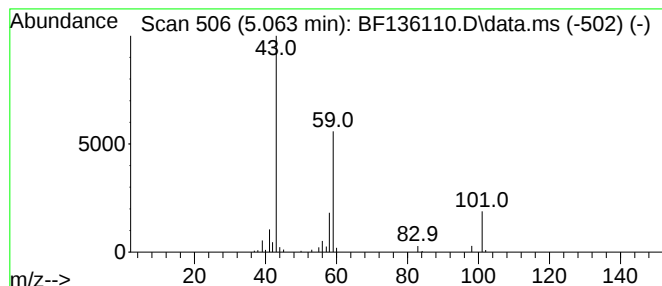
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	3.61 ng	107416	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32		
3	3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32		
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12		
5	Acetone	58	C3H6O	000067-64-1	9		



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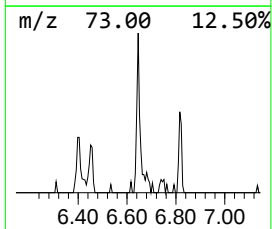
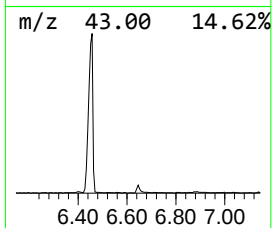
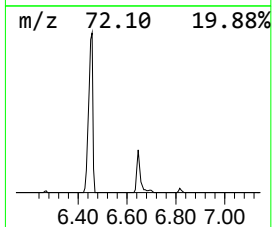
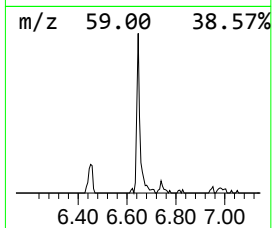
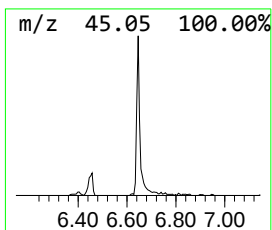
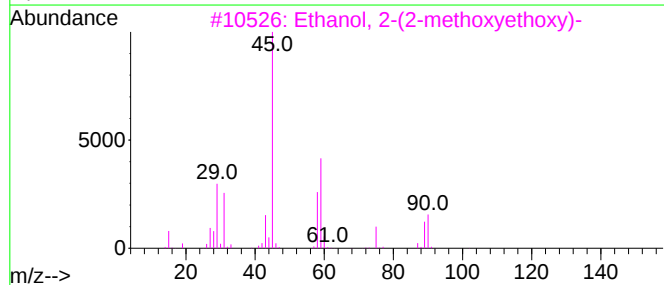
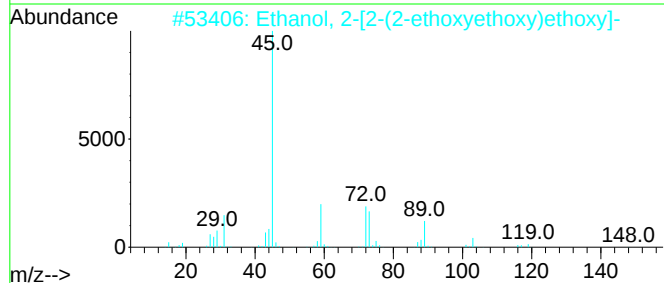
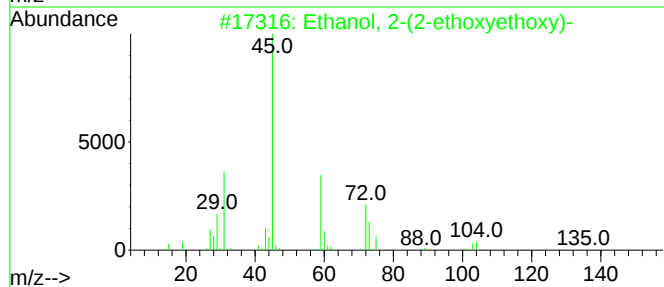
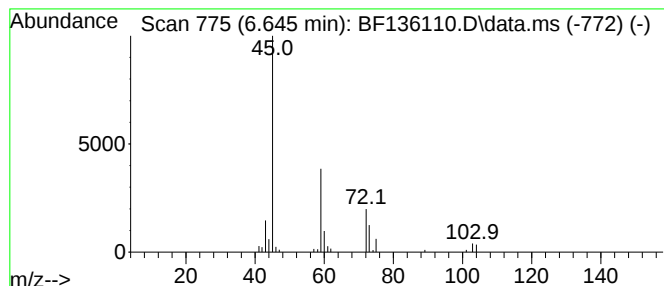
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.645	2.05 ng	60848	1,4-Dichlorobenzene-d4	6.816

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	83
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	53
3			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	45
4			Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	38
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	36



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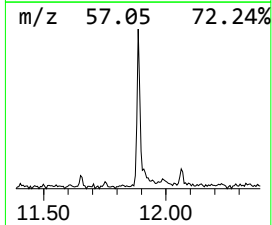
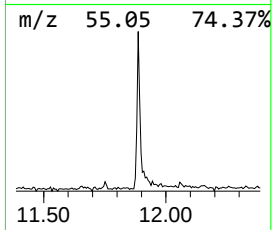
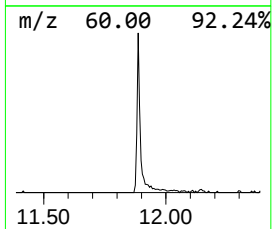
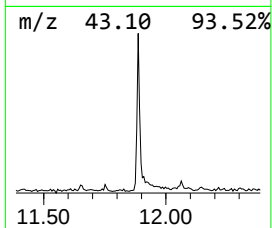
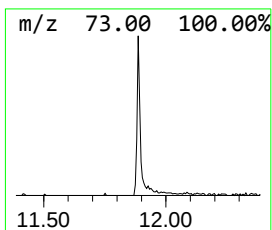
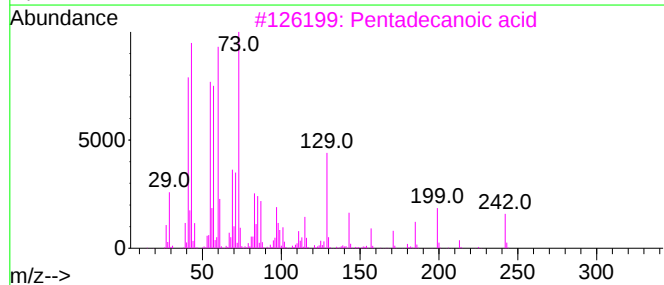
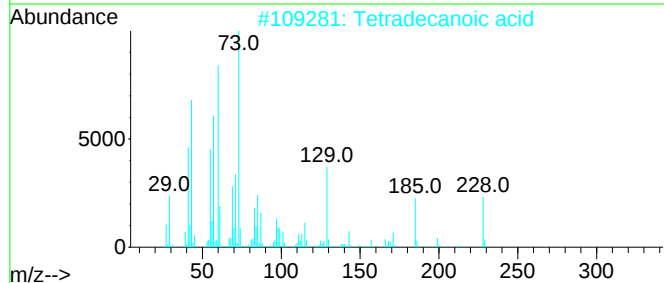
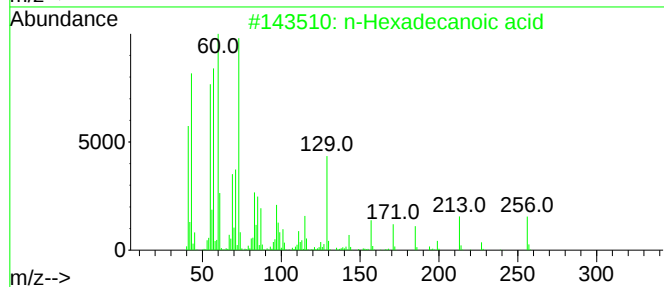
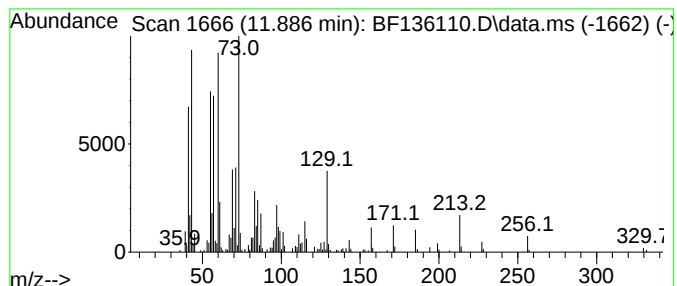
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.886	5.94 ng	226322	Phenanthrene-d10		11.345	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid		242	C15H30O2	001002-84-2	93
4	Tridecanoic acid		214	C13H26O2	000638-53-9	91
5	n-Decanoic acid		172	C10H20O2	000334-48-5	70



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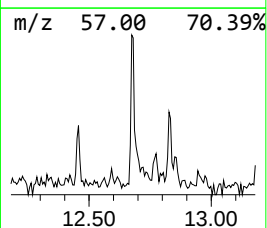
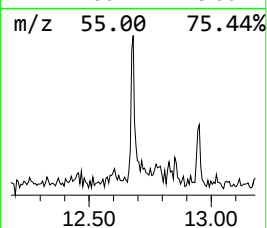
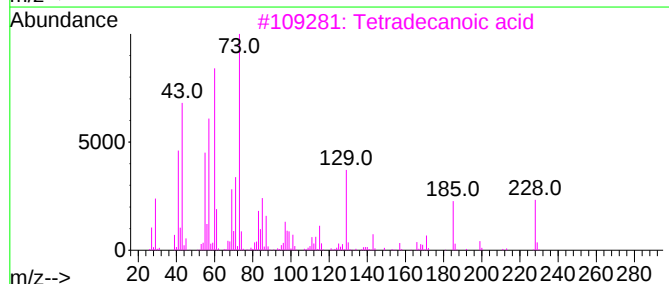
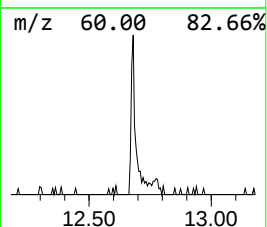
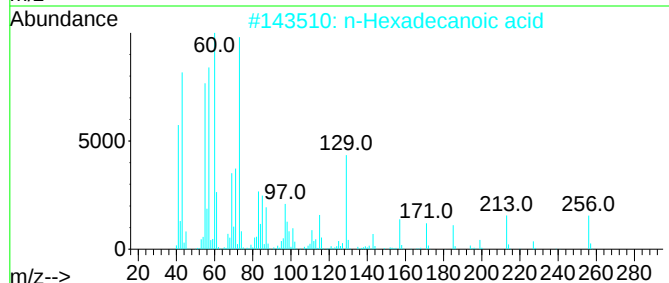
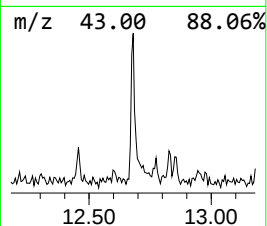
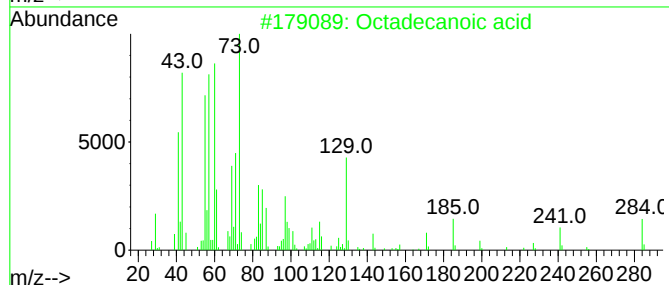
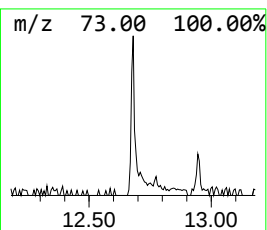
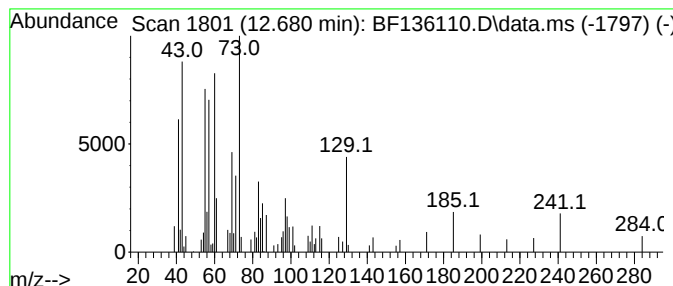
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.62 ng	71288	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	53



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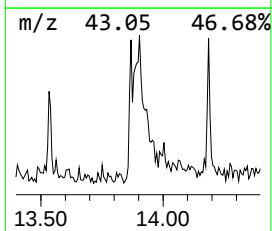
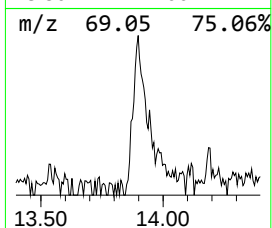
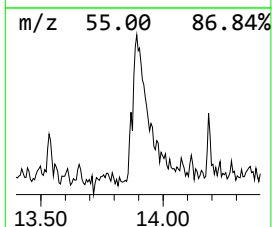
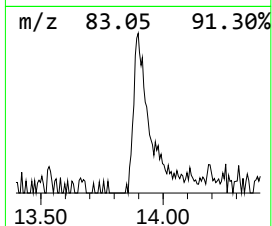
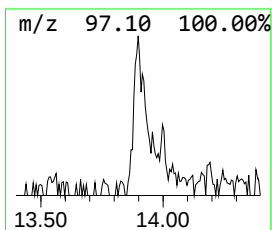
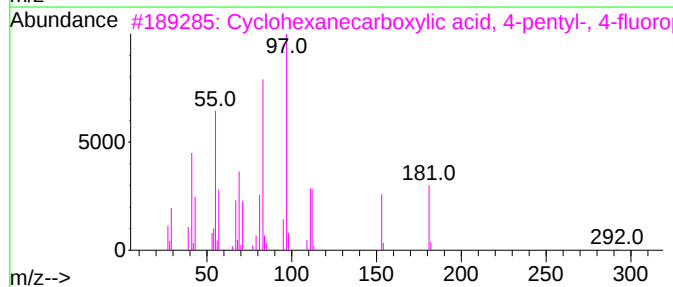
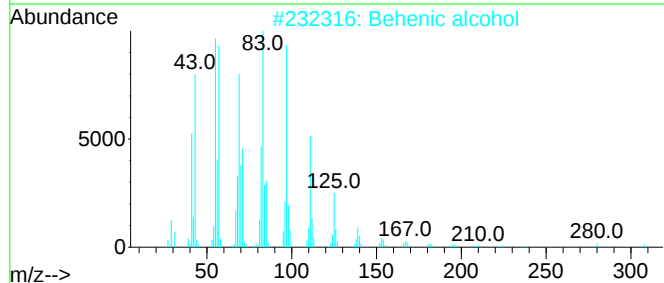
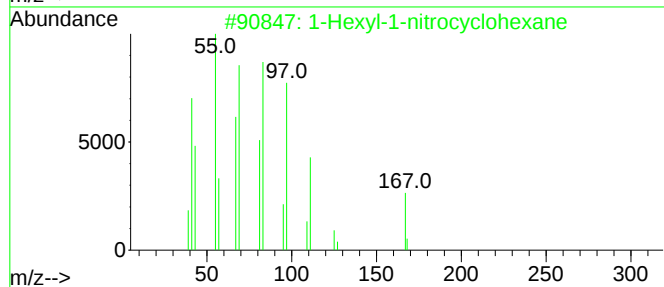
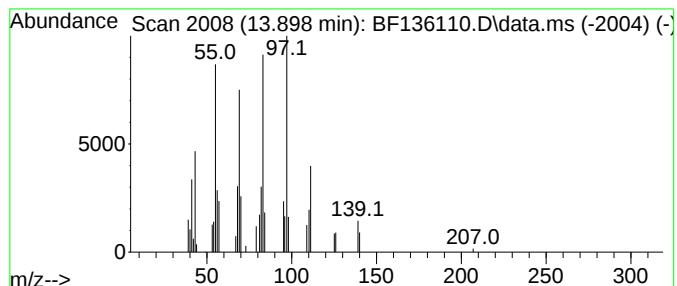
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Peak Number 5 1-Hexyl-1-nitrocyclohexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	2.38 ng	64746	Chrysene-d12	14.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexyl-1-nitrocyclohexane	213	C12H23NO2	118252-09-8	80
2			Behenic alcohol	326	C22H46O	000661-19-8	50
3			Cyclohexanecarboxylic acid, 4-pe...	292	C18H25FO2	079912-83-7	47
4			2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	43
5			2(5H)-Furanone, 5,5-dimethyl-	112	C6H8O2	020019-64-1	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.063	3.6	ng	107416	1	6.816	594474	20.0
Ethanol, 2-(2-e...	6.645	2.0	ng	60848	1	6.816	594474	20.0
n-Hexadecanoic ...	11.886	5.9	ng	226322	4	11.345	761469	20.0
Octadecanoic acid	12.680	2.6	ng	71288	5	14.004	544388	20.0
1-Hexyl-1-nitro...	13.898	2.4	ng	64746	5	14.004	544388	20.0