

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100622\
 Data File : BG055091.D
 Acq On : 6 Oct 2022 21:06
 Operator : CG/JU
 Sample : N5014-15
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-03-0-2.0

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_G\Methods\8270-BG100322.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055091.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.371	9	14	29	rVB	259741	408110	23.94%	4.804%
2	5.381	348	356	363	rBV	115958	175415	10.29%	2.065%
3	5.851	430	436	445	rVB	348086	557146	32.68%	6.558%
4	7.460	703	710	718	rBV	367877	626156	36.72%	7.371%
5	8.336	852	859	865	rBV	87140	146406	8.59%	1.723%
6	9.505	1050	1058	1066	rBV	210133	375209	22.01%	4.417%
7	11.162	1333	1340	1348	rVB	118652	216063	12.67%	2.543%
8	13.571	1743	1750	1757	rVB	624869	928904	54.48%	10.934%
9	14.940	1976	1983	1991	rBV	224406	342929	20.11%	4.037%
10	16.415	2227	2234	2245	rBV	655917	959593	56.28%	11.295%
11	17.672	2442	2448	2454	rBV	332786	491433	28.82%	5.785%
12	18.524	2587	2593	2602	rBV	56636	92240	5.41%	1.086%
13	19.699	2785	2793	2798	rBV	18841	28002	1.64%	0.330%
14	19.781	2801	2807	2816	rBV5	19038	38403	2.25%	0.452%
15	20.063	2850	2855	2859	rVB	15314	23095	1.35%	0.272%
16	20.251	2881	2887	2893	rBV	1292204	1705015	100.00%	20.070%
17	21.567	3106	3111	3119	rBV2	72033	111816	6.56%	1.316%
18	21.967	3171	3179	3185	rBV	335970	574482	33.69%	6.762%
19	22.813	3318	3323	3330	rBV7	11548	25945	1.52%	0.305%
20	24.429	3594	3598	3605	rVB2	15176	28694	1.68%	0.338%
21	25.416	3754	3766	3785	rBV2	188729	579985	34.02%	6.827%
22	26.714	3975	3987	3997	rBV5	17522	60353	3.54%	0.710%

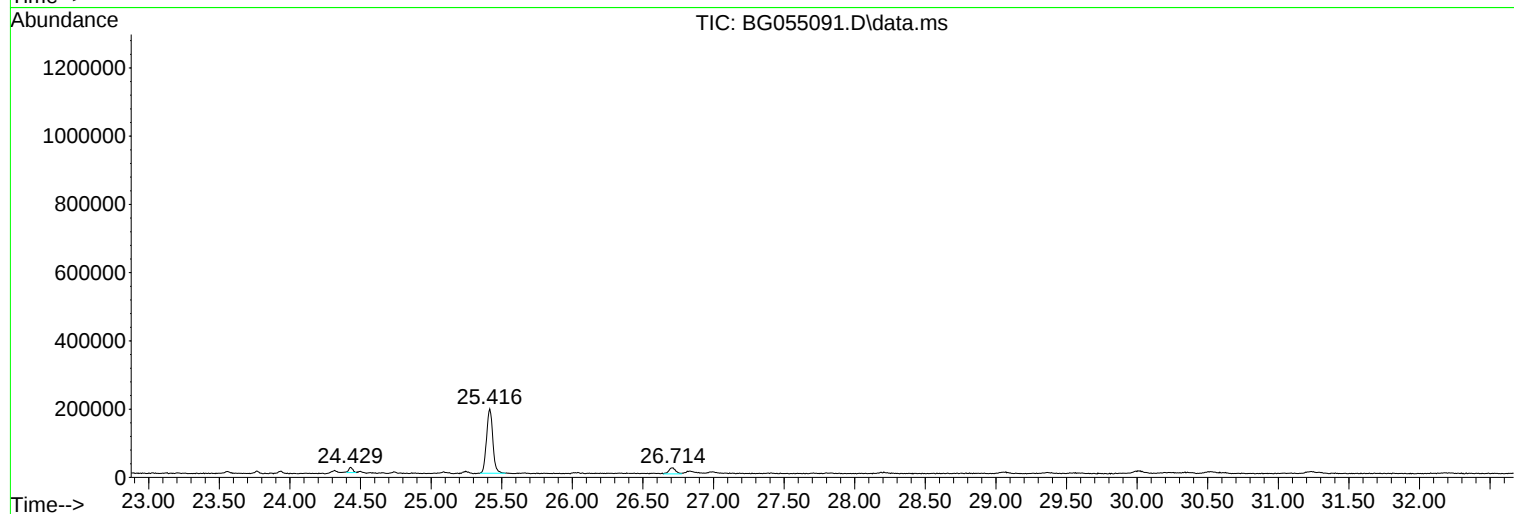
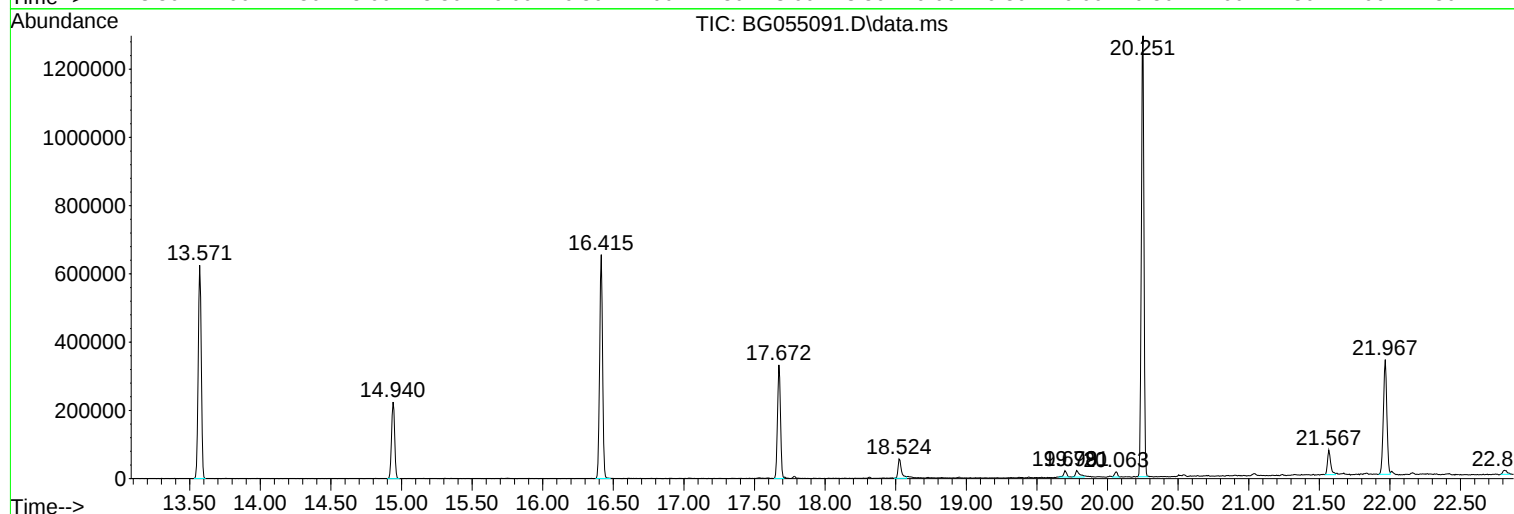
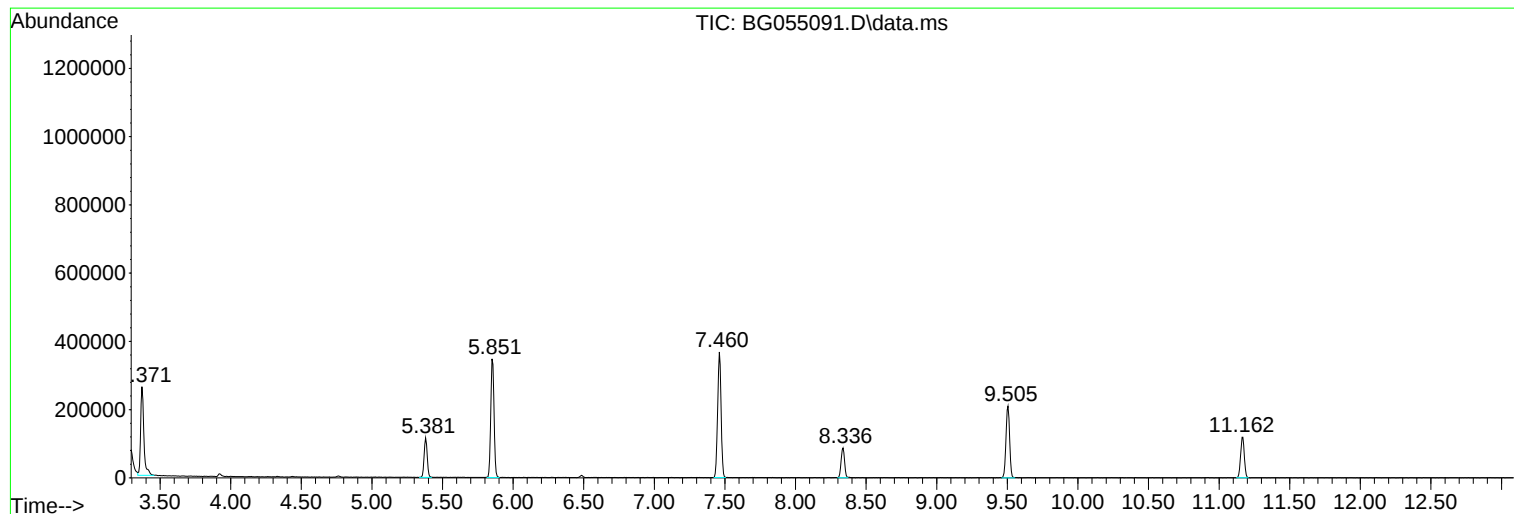
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Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG100322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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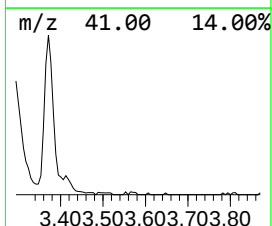
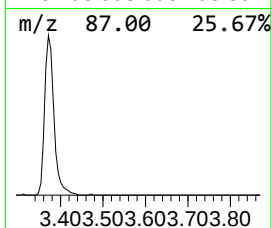
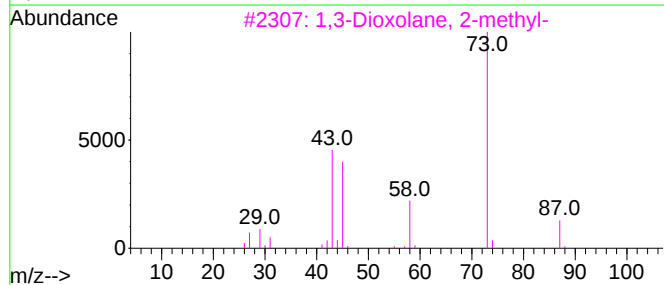
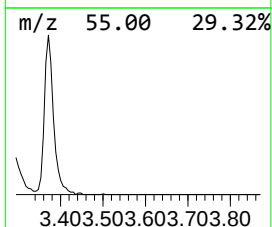
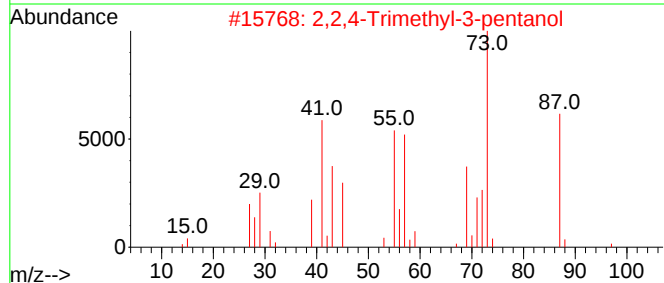
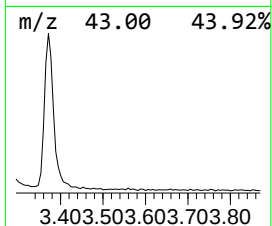
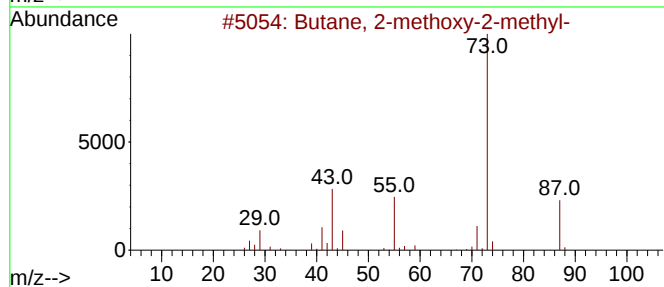
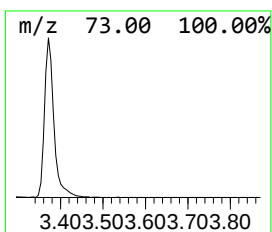
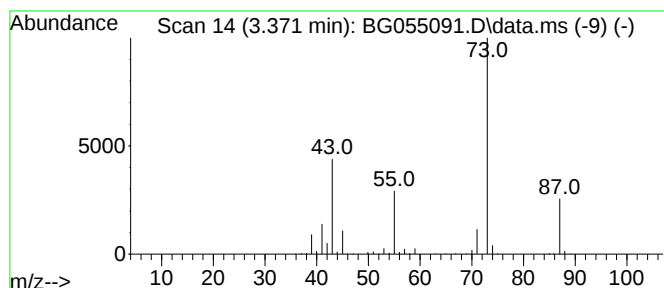
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.371	55.75 ng	408110	1,4-Dichlorobenzene-d4	8.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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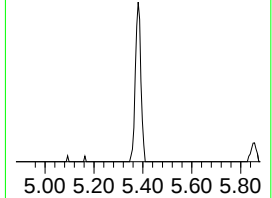
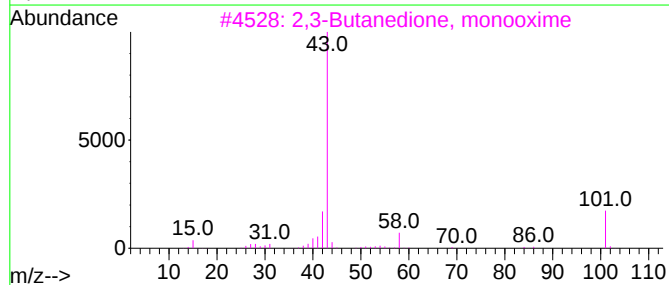
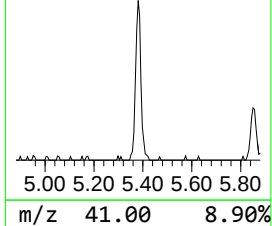
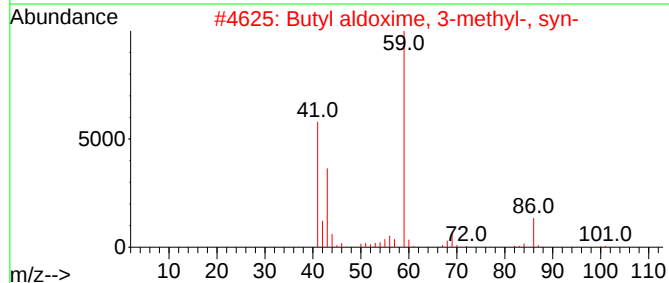
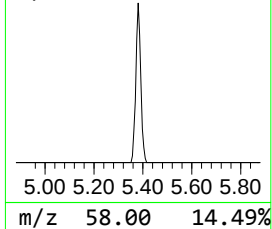
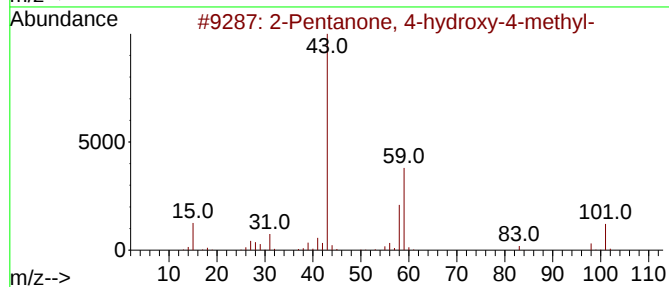
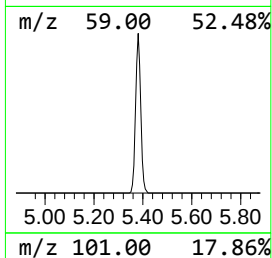
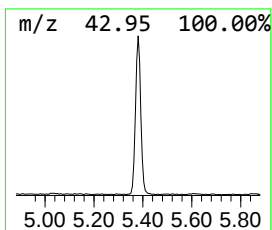
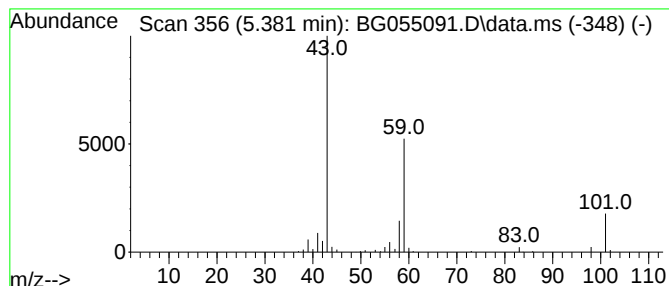
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.381	23.96 ng	175415	1,4-Dichlorobenzene-d4	8.336

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	12
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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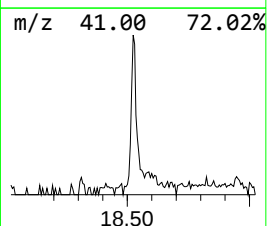
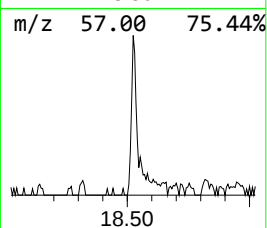
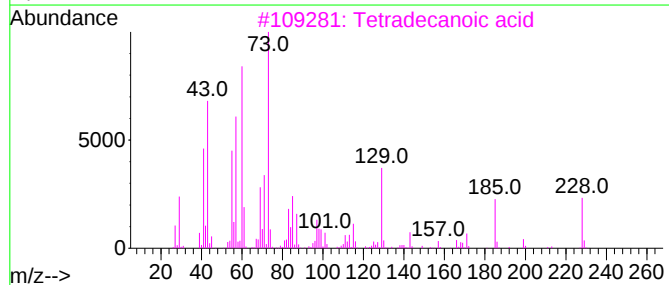
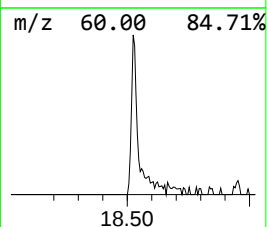
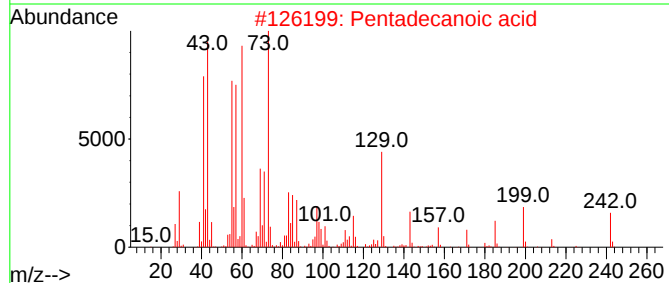
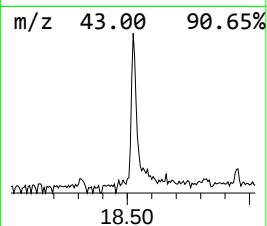
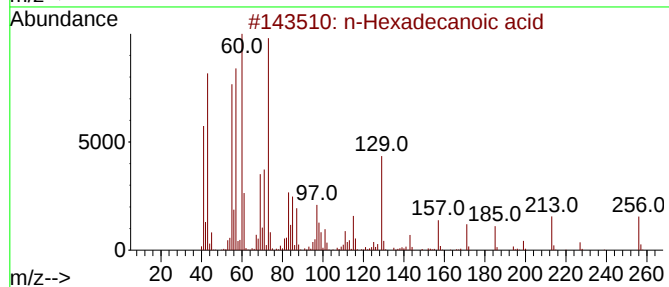
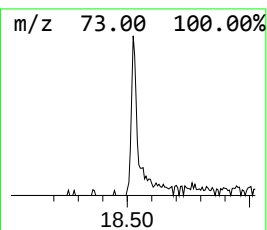
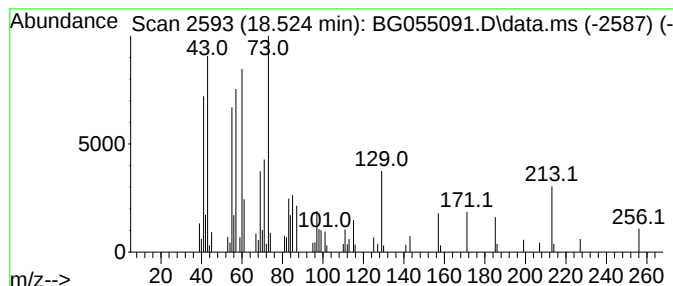
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.524	3.75 ng	92240	Phenanthrene-d10	17.672

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	76
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



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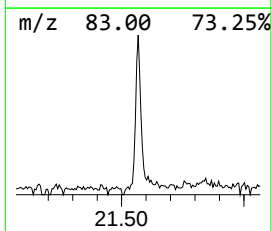
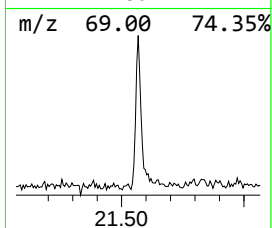
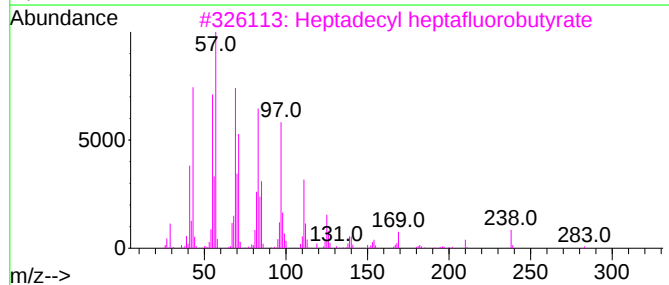
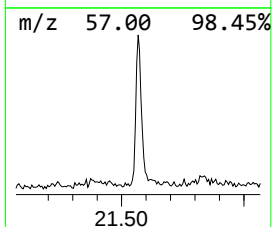
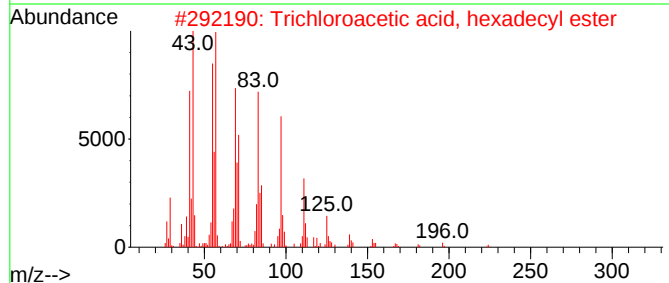
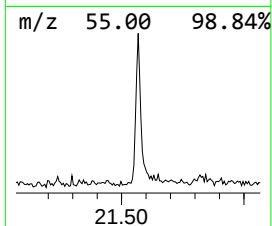
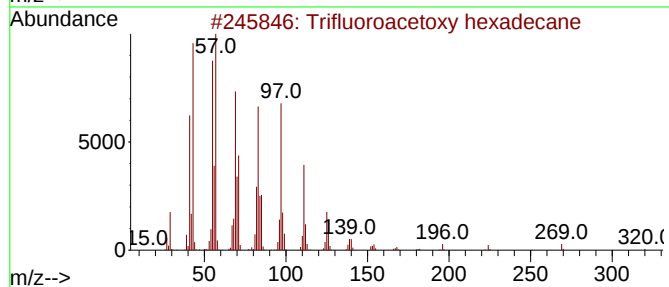
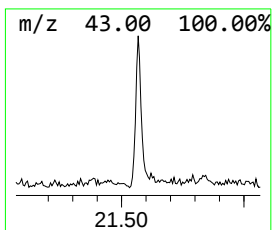
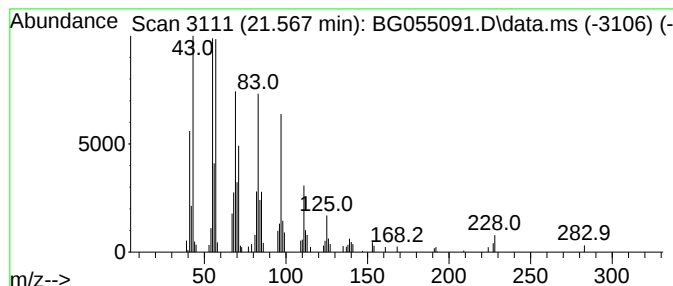
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.567	3.89 ng	111816	Chrysene-d12	21.967

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	95
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	95
4			Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	95
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95



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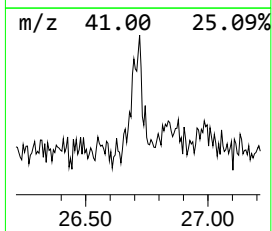
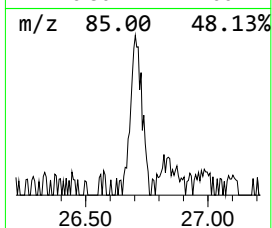
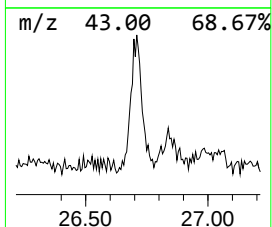
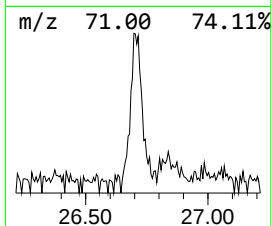
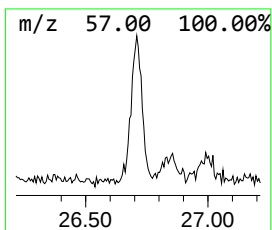
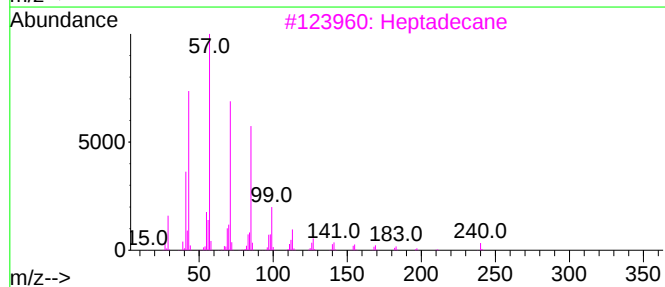
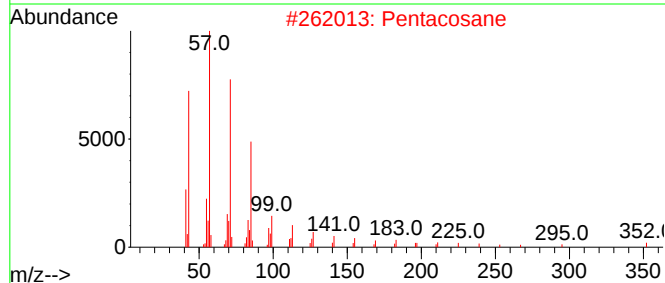
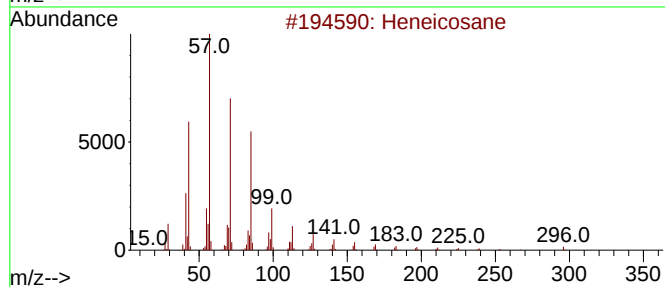
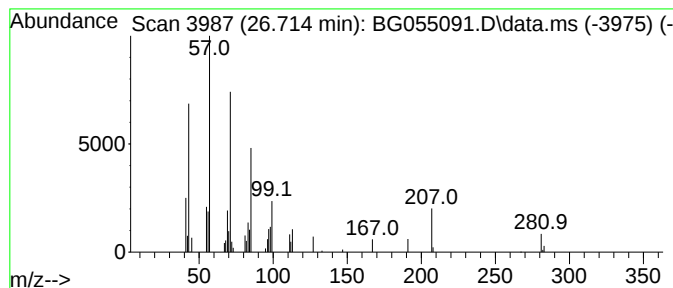
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.714	2.08 ng	60353	Perylene-d12	25.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heneicosane	296	C21H44	000629-94-7	80
2			Pentacosane	352	C25H52	000629-99-2	80
3			Heptadecane	240	C17H36	000629-78-7	80
4			Hexacosane	366	C26H54	000630-01-3	72
5			Hentriacontane	437	C31H64	000630-04-6	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.371	55.8	ng	408110	1	8.336	146406	20.0
2-Pentanone, 4-...	5.381	24.0	ng	175415	1	8.336	146406	20.0
n-Hexadecanoic ...	18.524	3.8	ng	92240	4	17.672	491433	20.0
Trifluoroacetox...	21.567	3.9	ng	111816	5	21.967	574482	20.0
Heneicosane	26.714	2.1	ng	60353	6	25.416	579985	20.0