

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010323\
 Data File : BG056196.D
 Acq On : 3 Jan 2023 21:48
 Operator : CG/JU
 Sample : N6233-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RO-124019

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-BG122722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG056196.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.366	7	13	22	rBV	100744	190374	7.00%	1.301%
2	5.382	346	356	363	rBV	148830	239282	8.79%	1.636%
3	5.863	430	438	452	rVB	654054	1072851	39.42%	7.334%
4	7.479	704	713	724	rBV	666984	1157245	42.52%	7.911%
5	8.343	851	860	870	rBB	198507	339117	12.46%	2.318%
6	9.512	1051	1059	1068	rBV	403726	711638	26.15%	4.865%
7	11.175	1334	1342	1354	rVB	256100	470902	17.30%	3.219%
8	13.578	1743	1751	1759	rBV	1326058	2045520	75.16%	13.984%
9	14.947	1976	1984	1991	rBV2	478913	748791	27.51%	5.119%
10	16.286	2206	2212	2215	rBV2	23852	31368	1.15%	0.214%
11	16.428	2229	2236	2244	rVB	958590	1455971	53.50%	9.954%
12	16.610	2261	2267	2275	rBV	75193	116684	4.29%	0.798%
13	17.685	2444	2450	2456	rBV	591540	911918	33.51%	6.234%
14	18.531	2589	2594	2602	rBV	149373	205911	7.57%	1.408%
15	19.782	2803	2807	2811	rBV6	41589	54488	2.00%	0.373%
16	20.258	2882	2888	2893	rBV	2169109	2721564	100.00%	18.606%
17	21.563	3106	3110	3116	rBV2	100959	155559	5.72%	1.063%
18	21.980	3175	3181	3189	rVB	554437	974942	35.82%	6.665%
19	25.446	3762	3771	3784	rVB2	344619	1023512	37.61%	6.997%

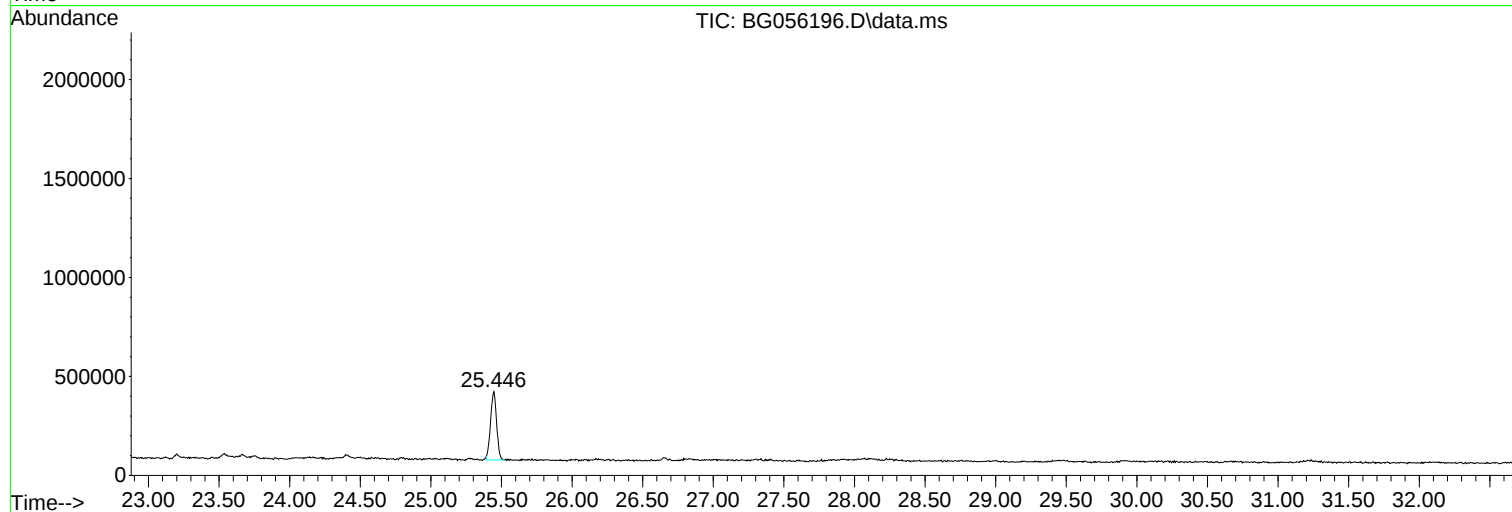
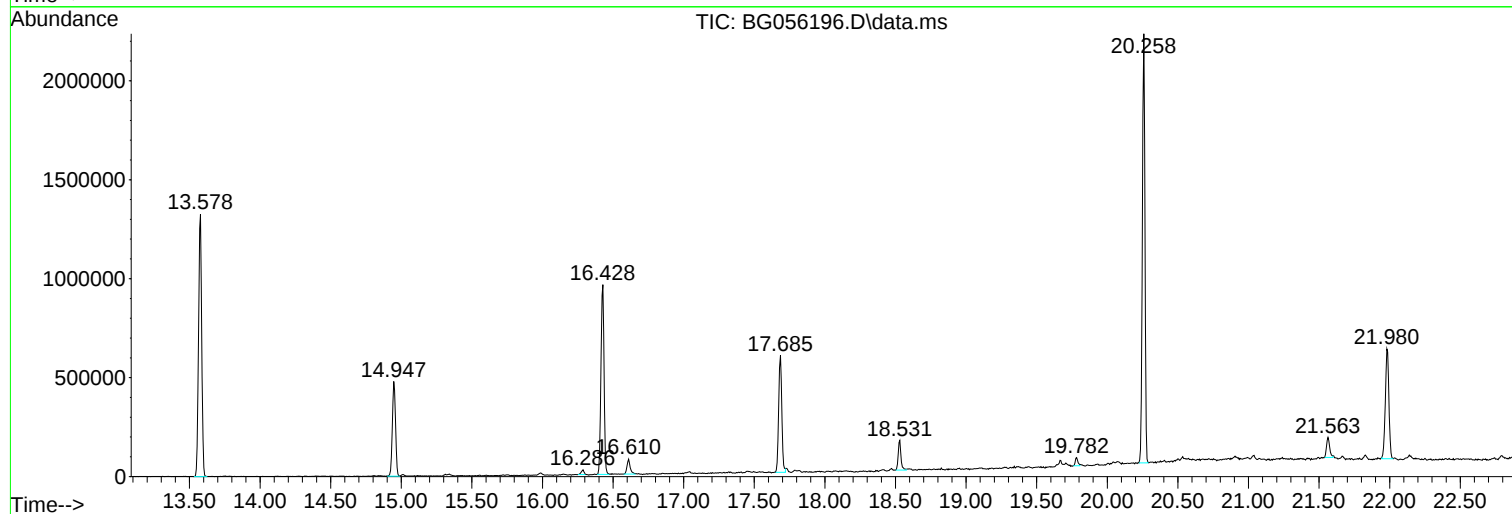
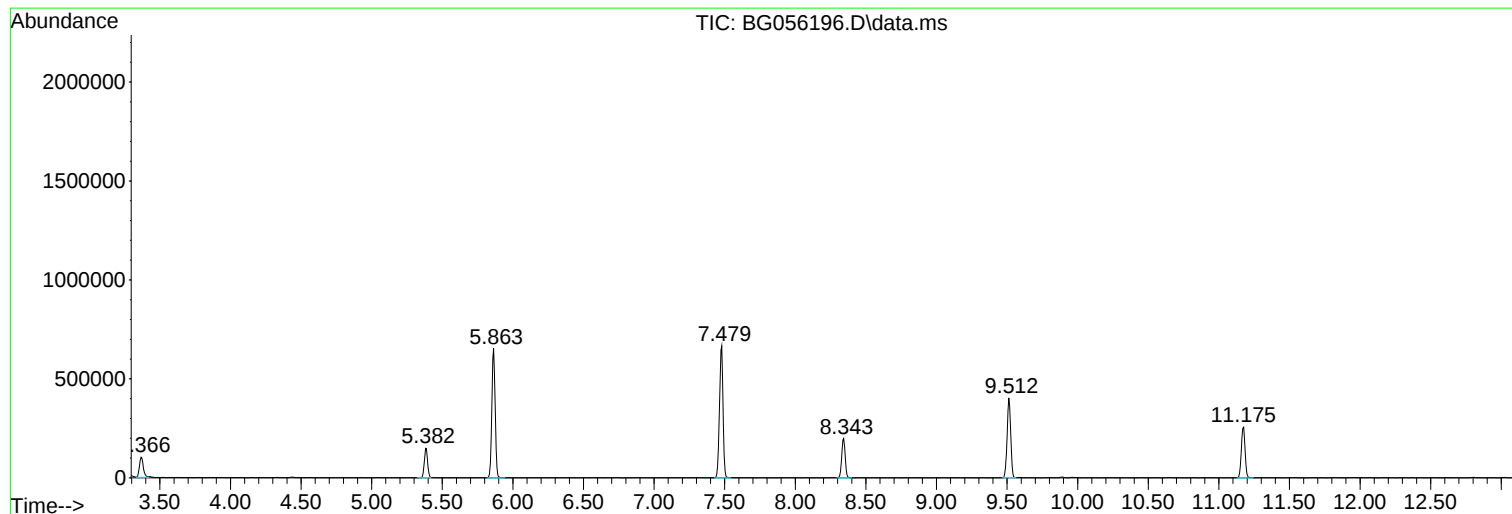
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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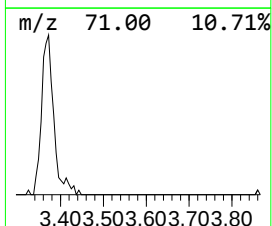
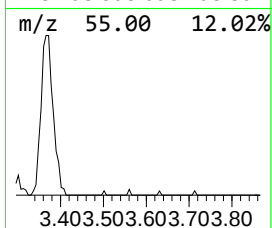
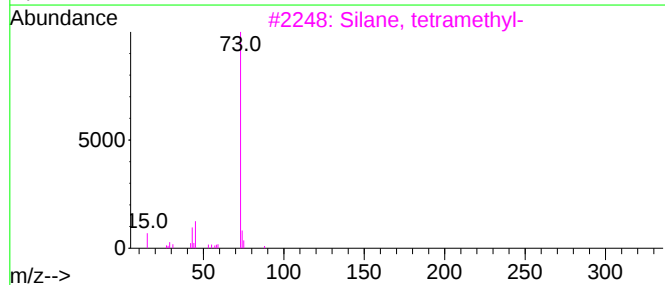
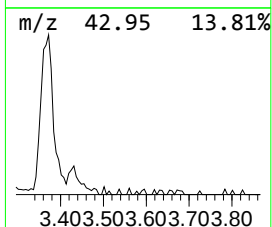
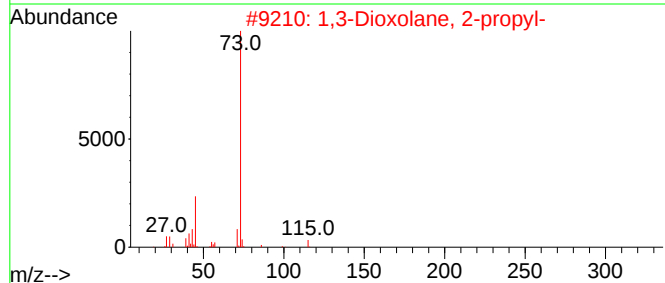
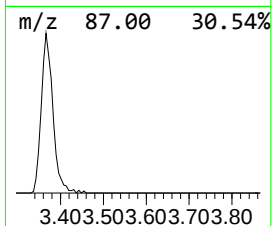
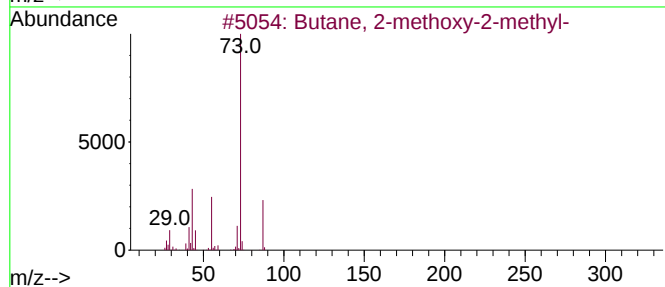
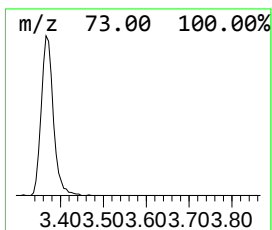
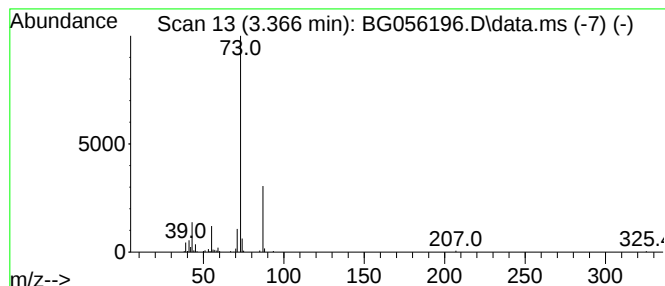
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.366	11.23 ng	190374	1,4-Dichlorobenzene-d4	8.343

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
3			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4			1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9



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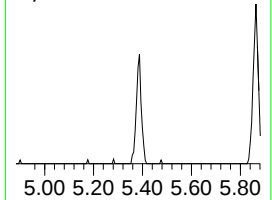
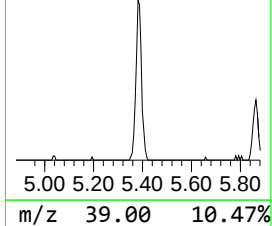
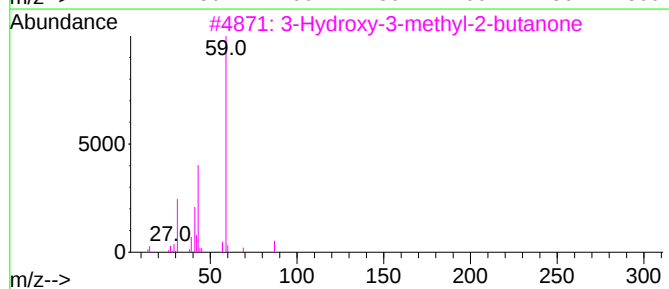
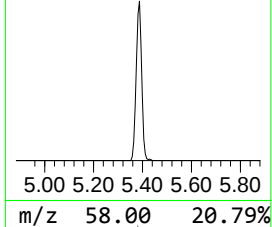
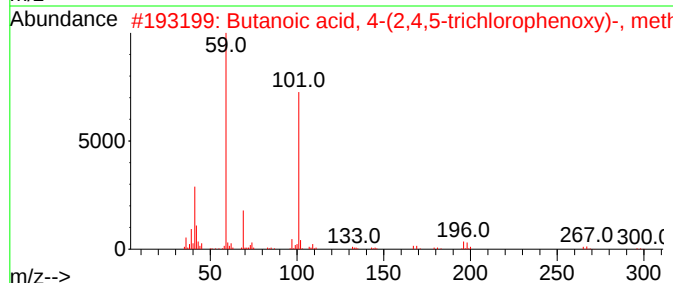
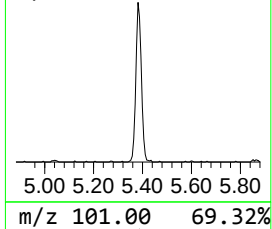
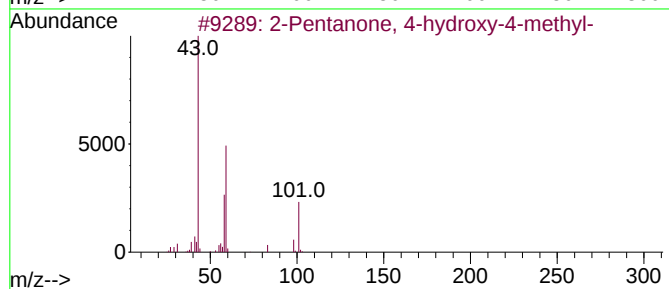
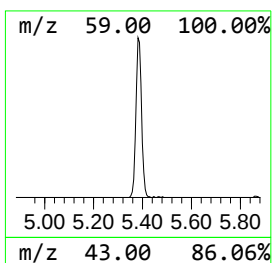
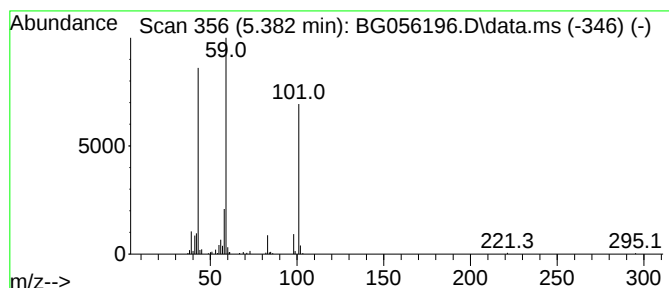
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.382	14.11 ng	239282	1,4-Dichlorobenzene-d4	8.343

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2			Butanoic acid, 4-(2,4,5-trichlor...	296	C11H11Cl3O3	025333-21-5	36
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	32
4			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	27
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	25



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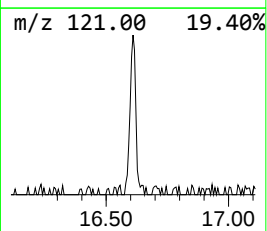
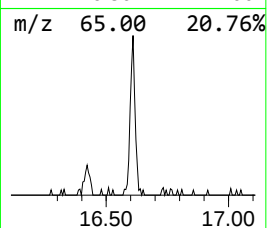
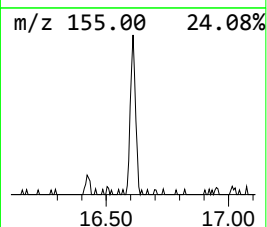
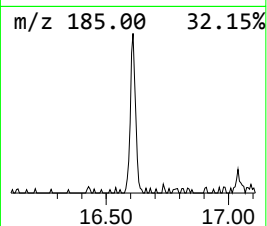
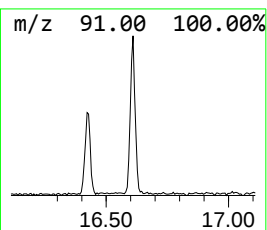
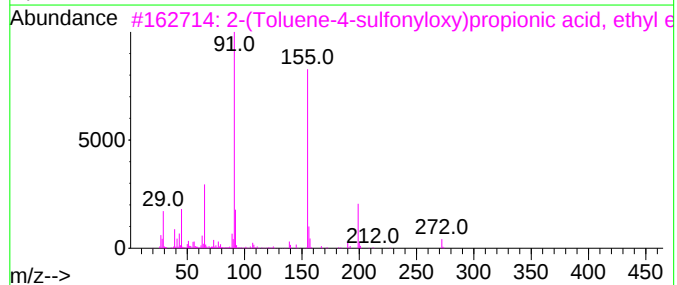
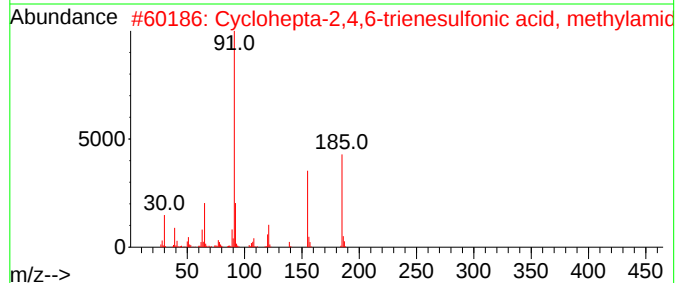
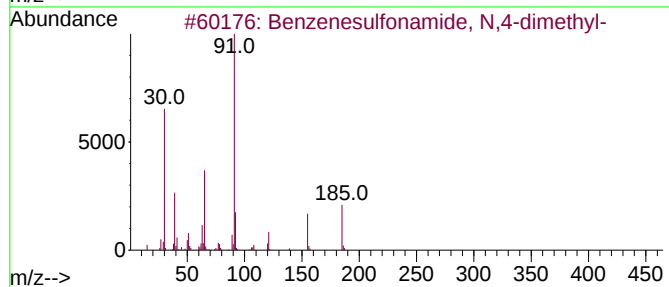
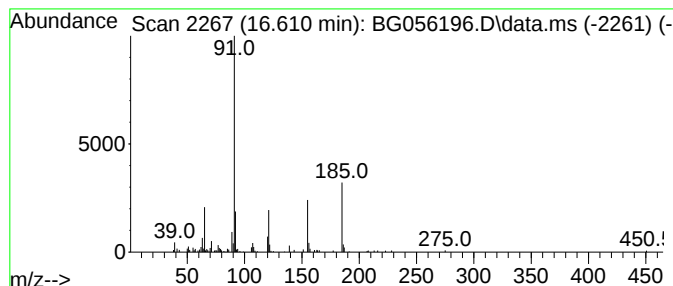
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Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.610	2.56 ng	116684	Phenanthrene-d10	17.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	93
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	76
3			2-(Toluene-4-sulfonyloxy)propion...	272	C12H16O5S	033798-77-5	53
4			3-Methyl-2-(toluene-4-sulfonylam...	283	C13H17NO4S	1000185-42-0	53
5			benzenesulfonamide, N-(cyanometh...	224	C10H12N2O2S	1000400-88-5	53



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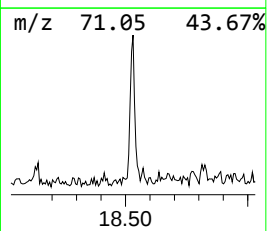
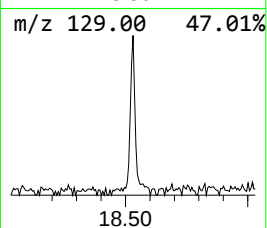
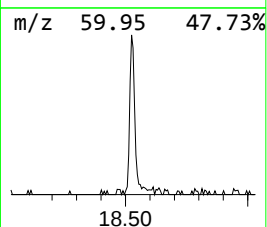
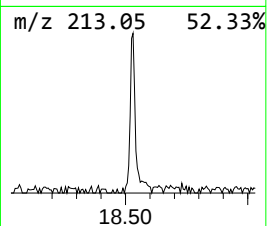
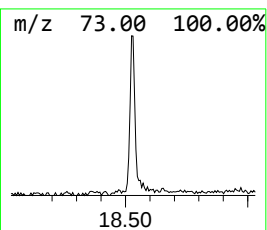
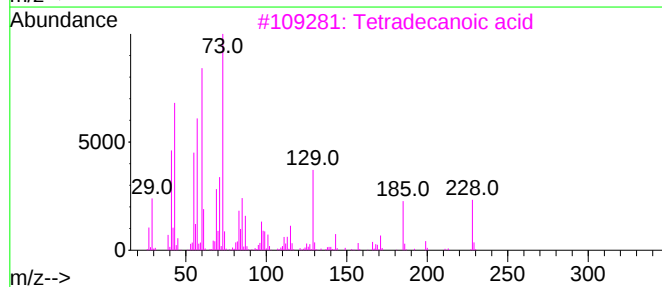
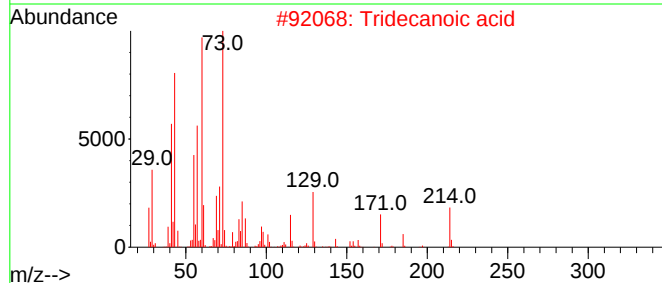
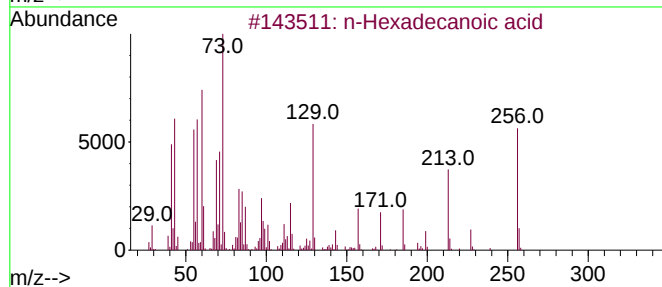
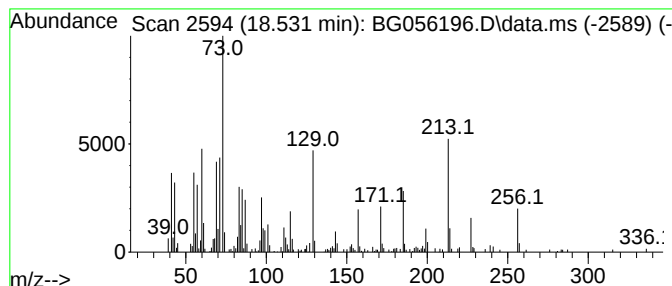
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.531	4.52 ng	205911	Phenanthrene-d10	17.685

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Tridecanoic acid	214	C13H26O2	000638-53-9	64
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	38
5			naphth[2,1-d]oxazole, 5-methoxy-...	213	C13H11NO2	1010396-17-7	20



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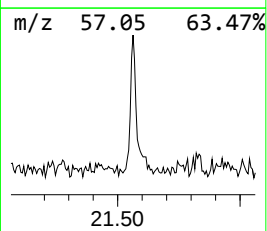
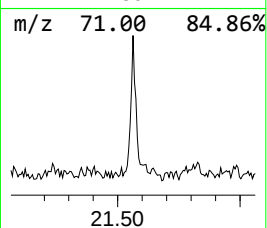
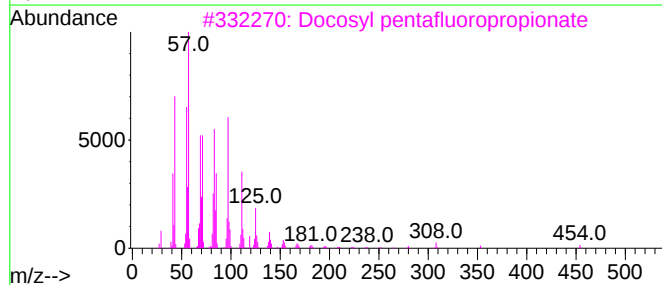
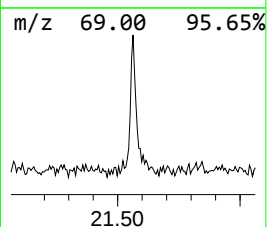
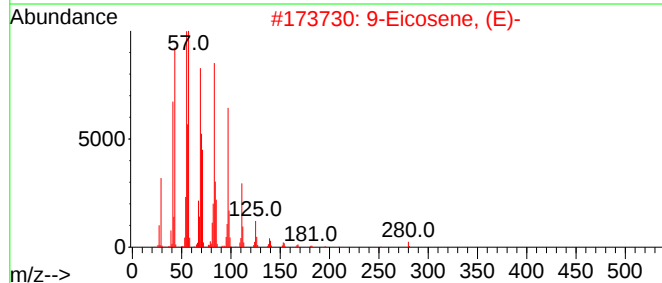
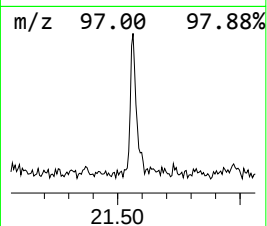
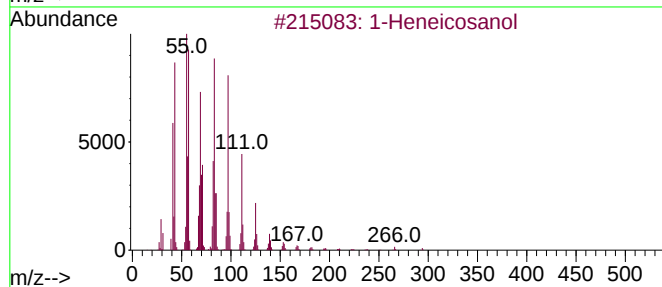
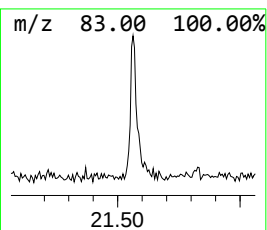
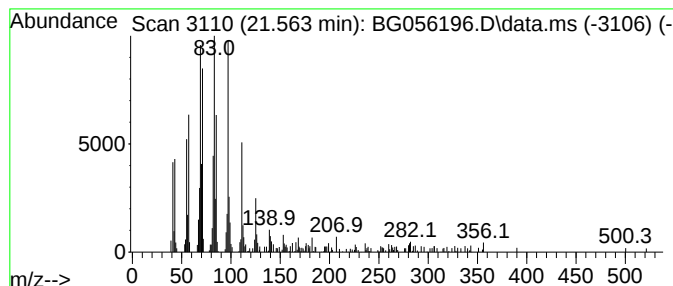
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.563	3.19 ng	155559	Chrysene-d12	21.980

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	81
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	81
3			Docosyl pentafluoropropionate	472	C25H45F5O2	1000351-80-9	81
4			Behenic alcohol	326	C22H46O	000661-19-8	80
5			5-Eicosene, (E)-	280	C20H40	074685-30-6	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.366	11.2	ng	190374	1	8.343	339117	20.0
2-Pentanone, 4-...	5.382	14.1	ng	239282	1	8.343	339117	20.0
Benzenesulfonam...	16.610	2.6	ng	116684	4	17.685	911918	20.0
n-Hexadecanoic ...	18.531	4.5	ng	205911	4	17.685	911918	20.0
1-Heneicosanol	21.563	3.2	ng	155559	5	21.980	974942	20.0