

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG010224\
 Data File : BG060191.D
 Acq On : 2 Jan 2024 12:29
 Operator : MA/JU
 Sample : 06039-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 EC48-EAST

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-BG122923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.118	3	5	10	rVB	359530	372745	2.67%	0.597%
2	5.039	327	332	338	rBV	247573	373469	2.68%	0.598%
3	5.509	405	412	430	rBV	2725765	4434105	31.82%	7.098%
4	5.926	475	483	494	rVB2	93610	169377	1.22%	0.271%
5	7.101	675	683	700	rBV	2518966	4550366	32.65%	7.284%
6	7.941	817	826	833	rBV	573070	1035783	7.43%	1.658%
7	9.099	1013	1023	1038	rBV	1388082	2487387	17.85%	3.981%
8	10.744	1295	1303	1311	rBV	828306	1520294	10.91%	2.433%
9	13.200	1714	1721	1735	rBV	4696307	7462423	53.55%	11.945%
10	14.022	1854	1861	1872	rBV	829638	1240324	8.90%	1.985%
11	14.575	1947	1955	1963	rBV	1673454	2673797	19.19%	4.280%
12	15.368	2084	2090	2097	rBV	1191928	1533663	11.01%	2.455%
13	16.061	2201	2208	2230	rBV2	3821641	5955620	42.74%	9.533%
14	17.324	2416	2423	2433	rBV	2555165	3976288	28.53%	6.365%
15	19.945	2863	2869	2880	rBV	10415996	13935450	100.00%	22.306%
16	21.238	3082	3089	3103	rBV	511741	925184	6.64%	1.481%
17	21.590	3142	3149	3159	rBV	2696714	4432046	31.80%	7.094%
18	23.041	3391	3396	3406	rBV6	82713	218336	1.57%	0.349%
19	23.253	3426	3432	3439	rVB	224261	413370	2.97%	0.662%
20	24.763	3679	3689	3703	rBV	1635169	4764144	34.19%	7.626%

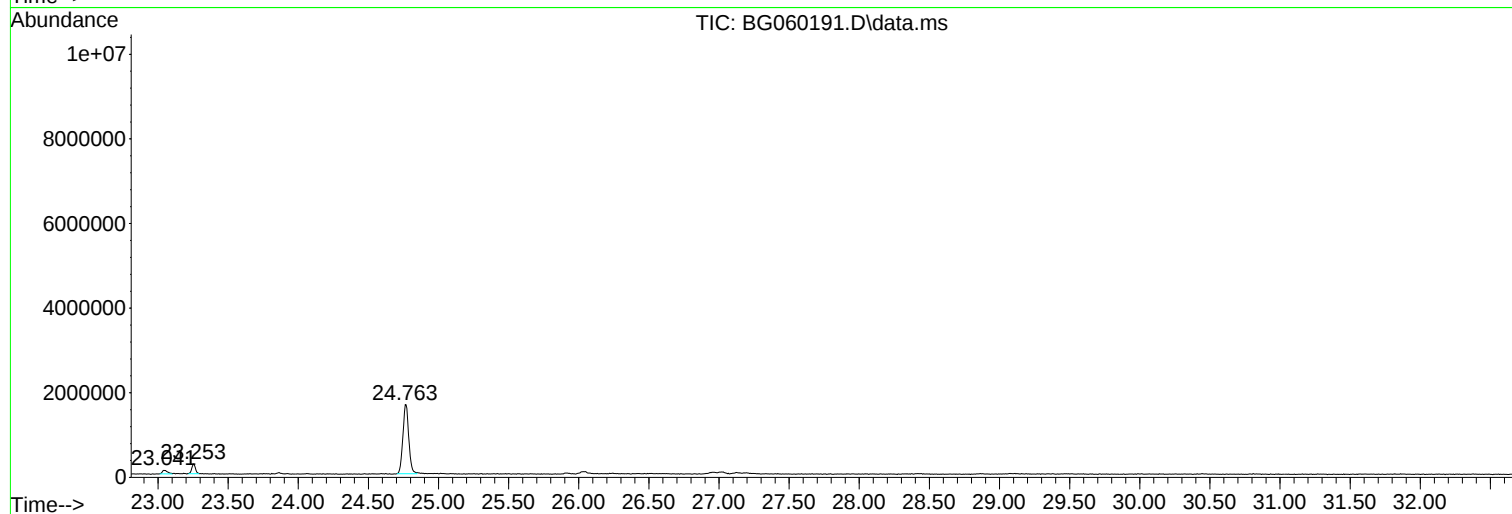
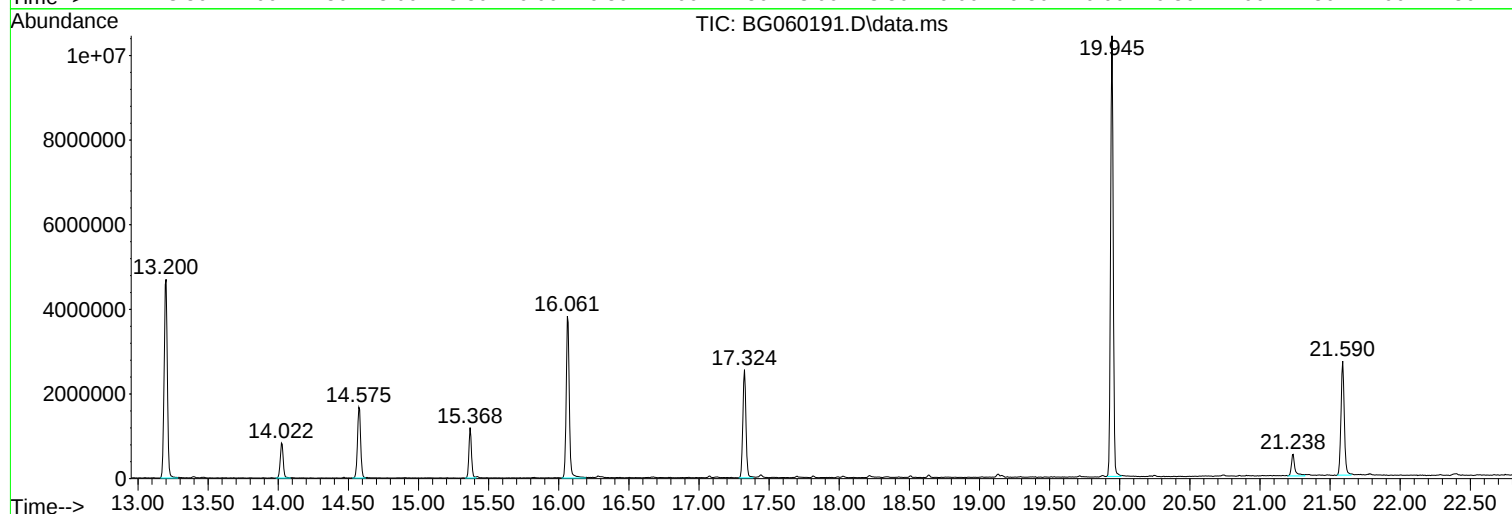
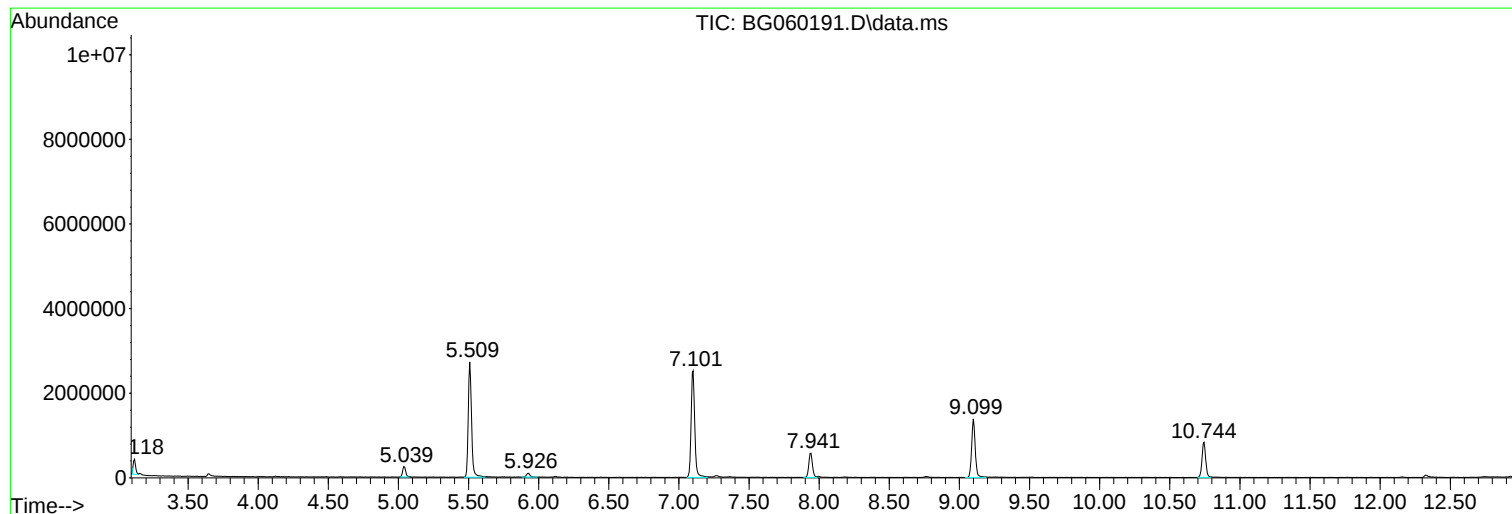
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG122923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : MA/JU
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Misc :
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Instrument :
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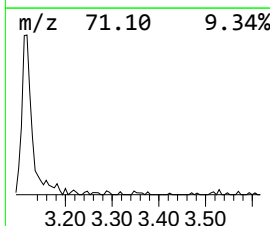
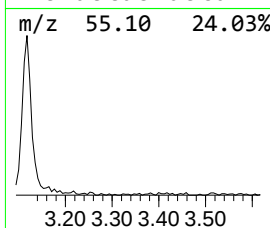
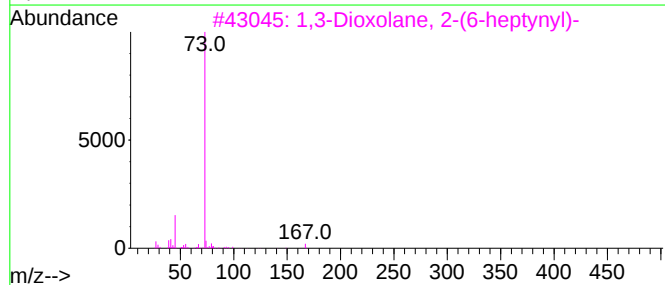
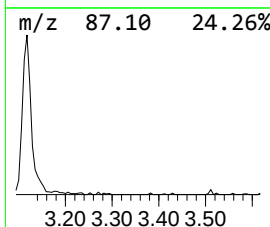
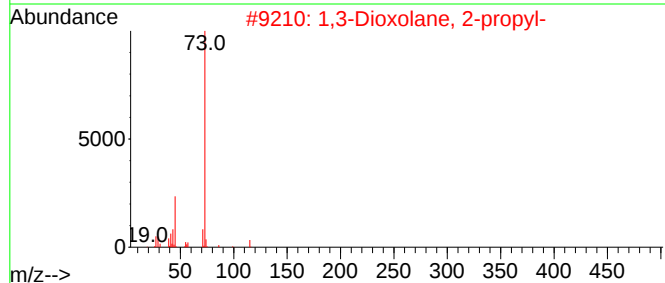
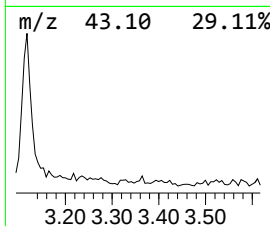
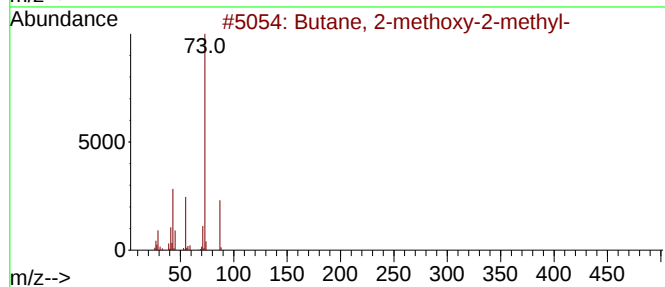
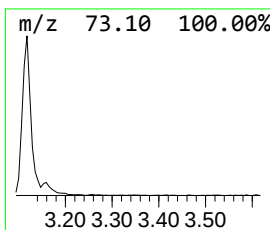
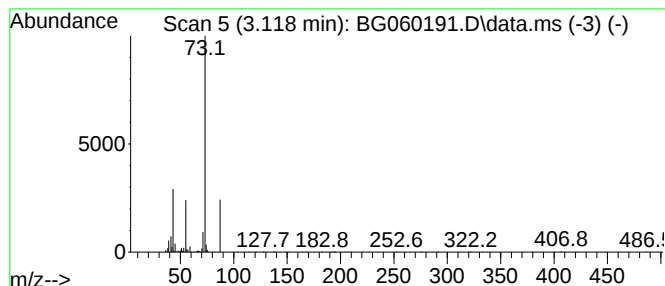
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.118 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.118	7.20 ng	372745	1,4-Dichlorobenzene-d4	7.941

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	45
2			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23
3			1,3-Dioxolane, 2-(6-heptynyl)-	168	C10H16O2	025595-82-8	9
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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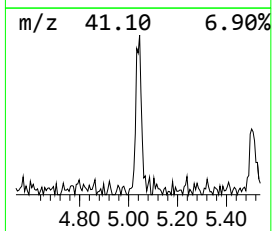
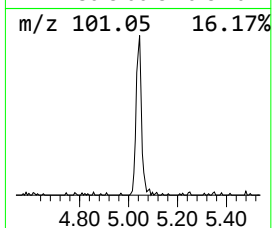
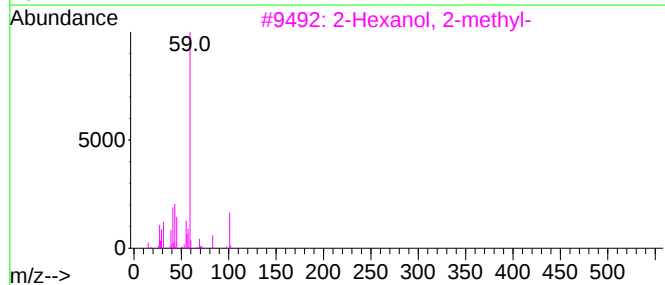
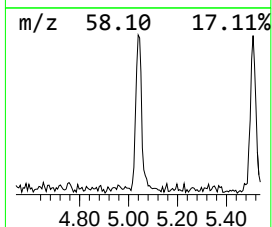
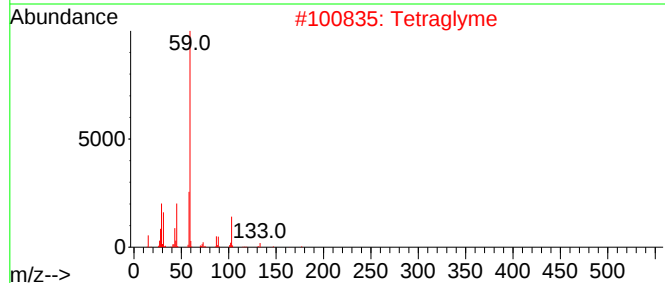
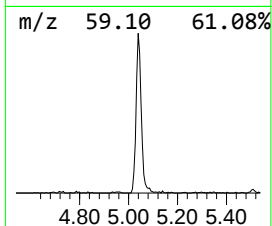
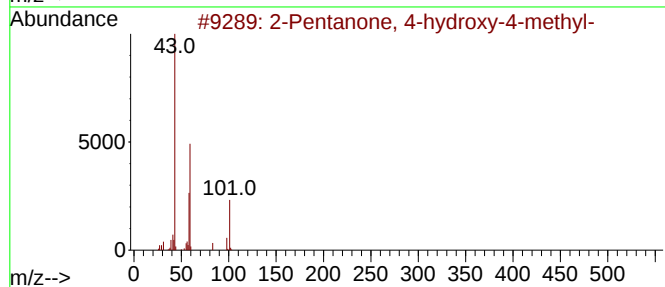
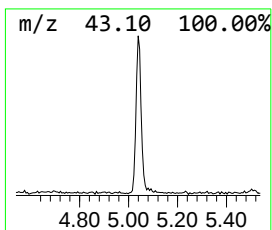
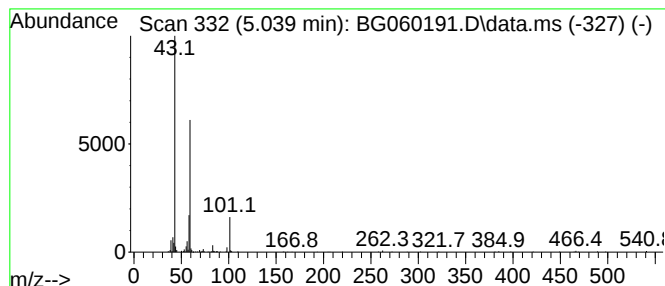
Instrument :
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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.039	7.21 ng	373469	1,4-Dichlorobenzene-d4			7.941
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	53
2	Tetraglyme		222	C10H22O5	000143-24-8	37
3	2-Hexanol, 2-methyl-		116	C7H16O	000625-23-0	25
4	3-Hexanol, 4-methyl-		116	C7H16O	000615-29-2	25
5	1,8-Nonanediol, 8-methyl-		174	C10H22O2	054725-73-4	23



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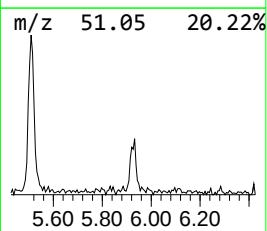
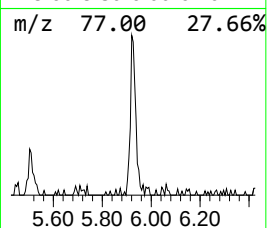
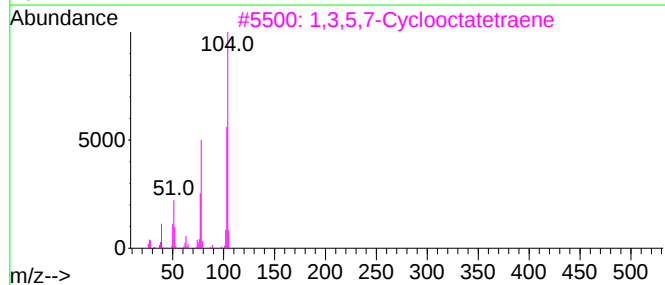
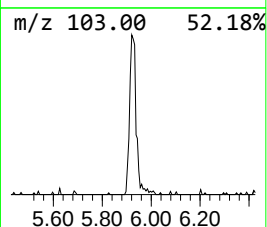
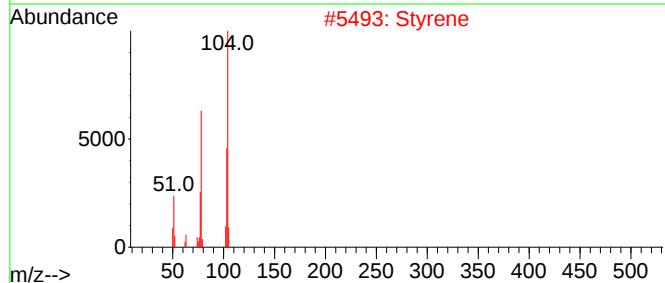
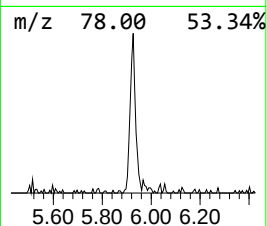
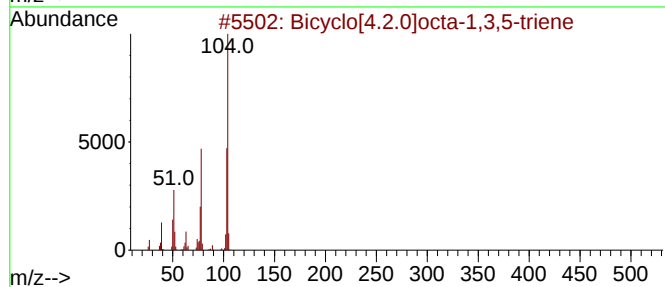
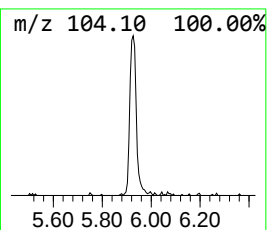
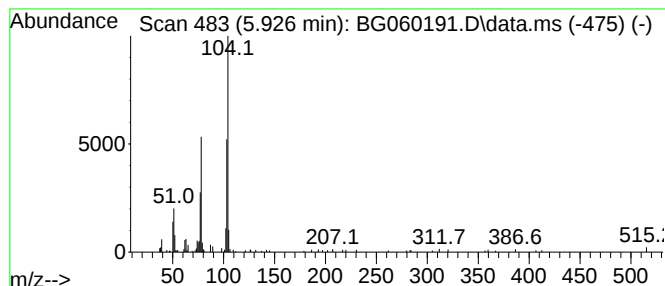
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BNA_G
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.926	3.27 ng	169377	1,4-Dichlorobenzene-d4	7.941	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	96
2	Styrene	104	C8H8	000100-42-5	95
3	1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	94
4	Benzeneethanamine, N-[(4-hydroxy...	269	C17H19NO2	106827-59-2	72
5	2-Propenoic acid, 3-phenyl-, 2-p...	252	C17H16O2	000103-53-7	53



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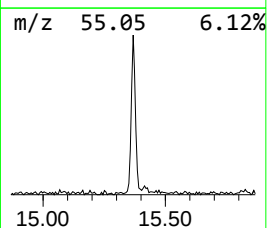
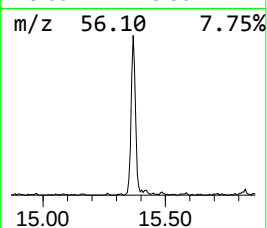
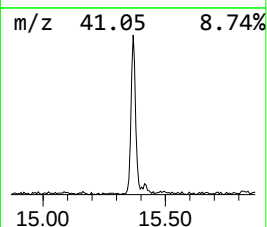
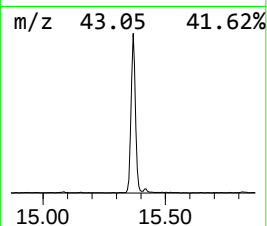
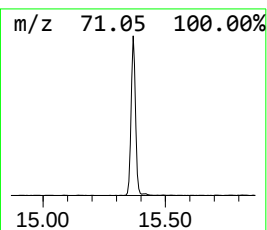
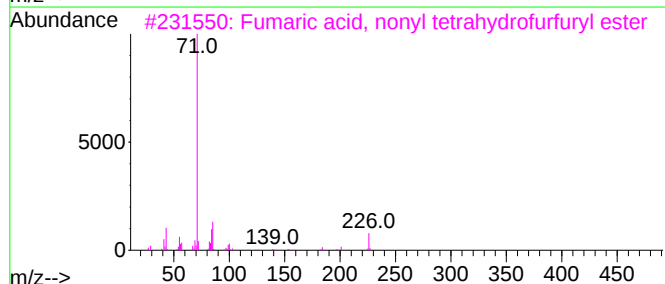
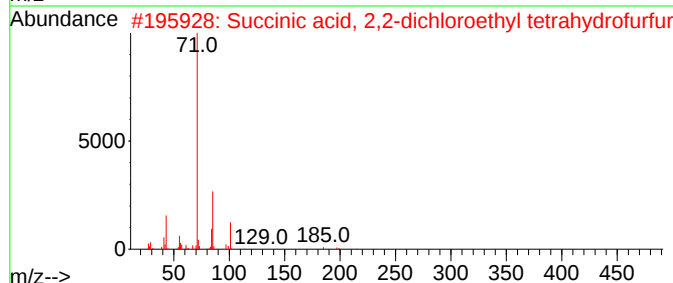
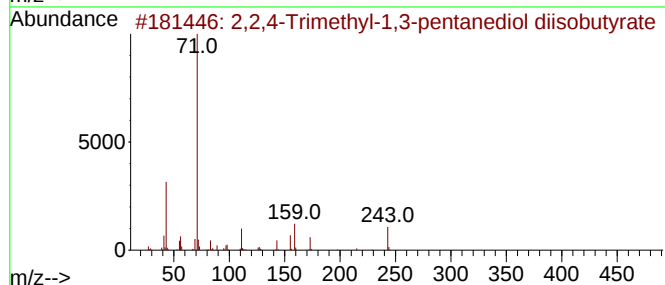
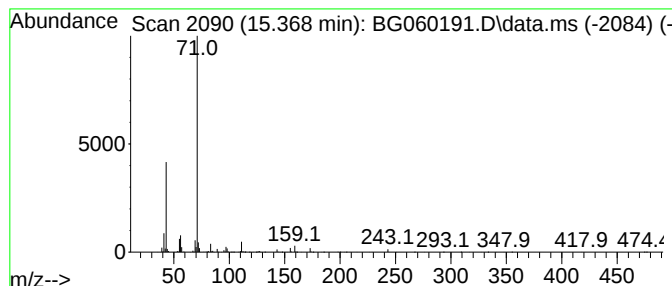
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Peak Number 4 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.368	11.47 ng	1533660	Acenaphthene-d10	14.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	74		
2	Succinic acid, 2,2-dichloroethyl...	298	C11H16Cl2O5	1000390-71-6	50		
3	Fumaric acid, nonyl tetrahydrofu...	326	C18H30O5	1000330-58-3	50		
4	Oxalic acid, decyl neopentyl ester	300	C17H32O4	1000309-73-4	40		
5	Sulfurous acid, dodecyl 2-pentyl...	320	C17H36O3S	1000309-16-1	40		



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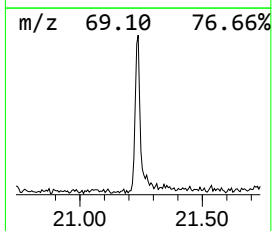
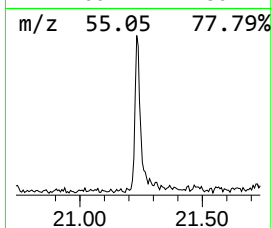
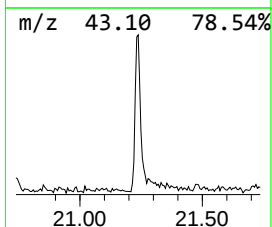
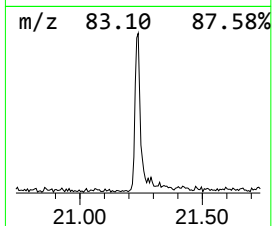
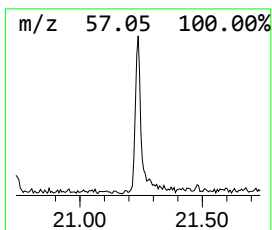
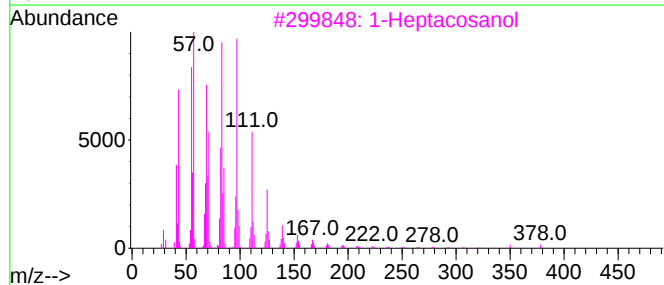
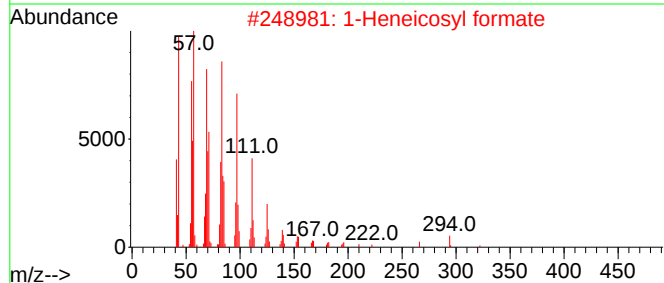
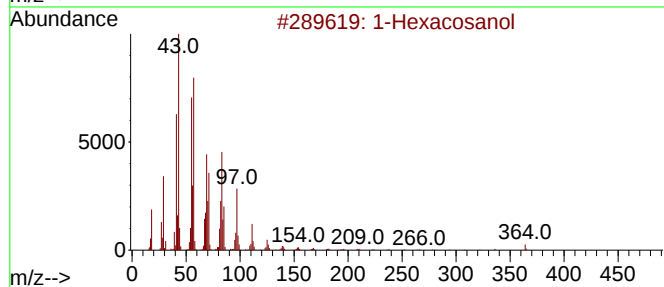
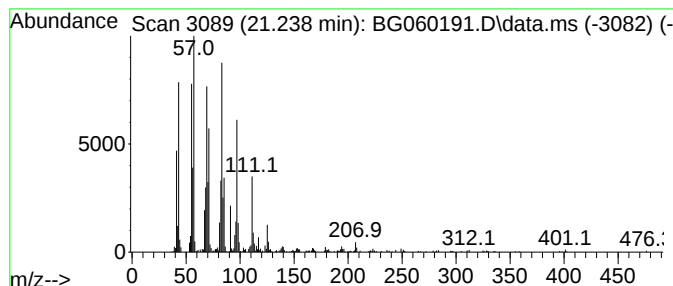
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 1-Hexacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.238	4.17 ng	925184	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexacosanol	382	C26H54O	000506-52-5	91
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
3			1-Heptacosanol	396	C27H56O	002004-39-9	91
4			Nonacos-1-ene	406	C29H58	018835-35-3	91
5			1-Hexacosene	364	C26H52	018835-33-1	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.118	3.118	7.2	ng	372745	1	7.941	1035780	20.0
2-Pentanone, 4-...	5.039	7.2	ng	373469	1	7.941	1035780	20.0
Bicyclo[4.2.0]o...	5.926	3.3	ng	169377	1	7.941	1035780	20.0
2,2,4-Trimethyl...	15.368	11.5	ng	1533660	3	14.575	2673800	20.0
1-Hexacosanol	21.238	4.2	ng	925184	5	21.590	4432050	20.0