

Data Path : Z:\SVOASRV\HPCHEM1\BNA P\DATA\BP122719\
 Data File : BP001476.D
 Acq On : 28 Dec 2019 00:16
 Operator : JU
 Sample : K6438-09
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 DUNR-BF006-01

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP121919.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.587	590	595	611	rVB	63183	97612	11.46%	1.618%
2	6.199	694	699	714	rBV	370888	500675	58.76%	8.299%
3	7.746	956	962	976	rBV	419787	545452	64.01%	9.041%
4	7.928	987	993	1005	rVB	479983	561432	65.89%	9.306%
5	8.281	1048	1053	1063	rVB	121133	139796	16.41%	2.317%
6	8.522	1088	1094	1107	rVB	388310	448684	52.66%	7.437%
7	9.163	1197	1203	1223	rBV	272850	347539	40.79%	5.761%
8	10.316	1394	1399	1418	rBV	122870	161763	18.98%	2.681%
9	12.093	1696	1701	1721	rBV	495080	654164	76.77%	10.843%
10	12.769	1811	1816	1828	rBV	10857	18272	2.14%	0.303%
11	13.181	1880	1886	1900	rBV	142582	200255	23.50%	3.319%
12	14.475	2100	2106	2126	rBV	350191	510594	59.92%	8.463%
13	15.575	2288	2293	2306	rBV	168815	222568	26.12%	3.689%
14	16.469	2440	2445	2455	rBV3	22068	33703	3.96%	0.559%
15	17.863	2676	2682	2697	rBV	805752	852083	100.00%	14.124%
16	19.139	2888	2899	2908	rBV5	26562	97775	11.47%	1.621%
17	19.222	2908	2913	2927	rVB	184485	235260	27.61%	3.900%
18	19.863	3009	3022	3025	rBV8	35416	108454	12.73%	1.798%
19	19.969	3036	3040	3048	rBV10	3794	9470	1.11%	0.157%
20	20.269	3088	3091	3097	rVB	11752	14090	1.65%	0.234%
21	20.663	3153	3158	3163	rBV	12680	16185	1.90%	0.268%
22	20.986	3207	3213	3224	rBV	138153	205838	24.16%	3.412%
23	21.092	3227	3231	3236	rVB2	10545	14790	1.74%	0.245%
24	21.586	3309	3315	3319	rBV3	10470	18610	2.18%	0.308%
25	21.727	3333	3339	3347	rBV3	5586	17994	2.11%	0.298%

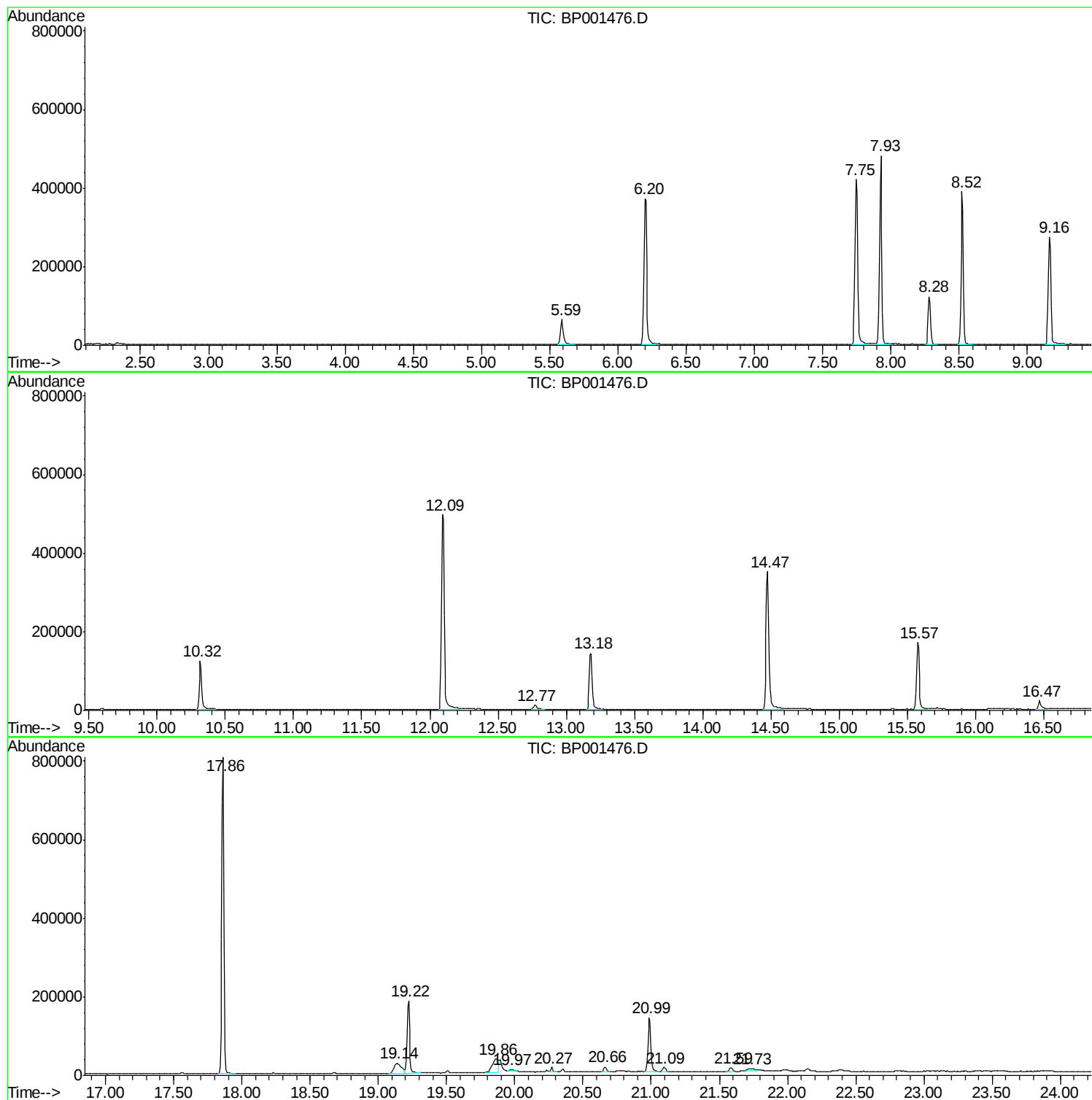
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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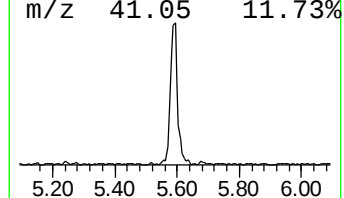
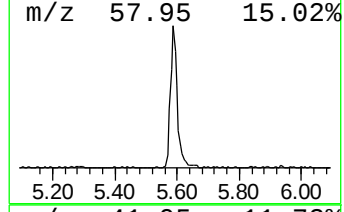
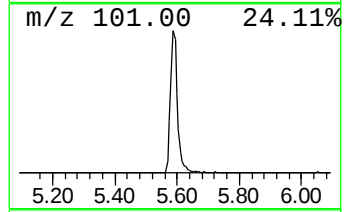
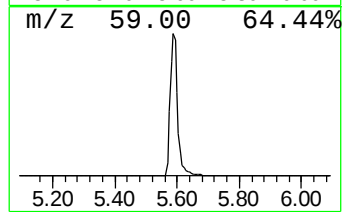
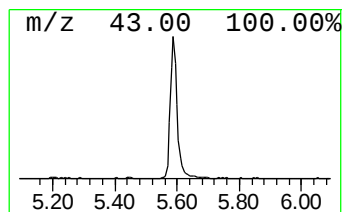
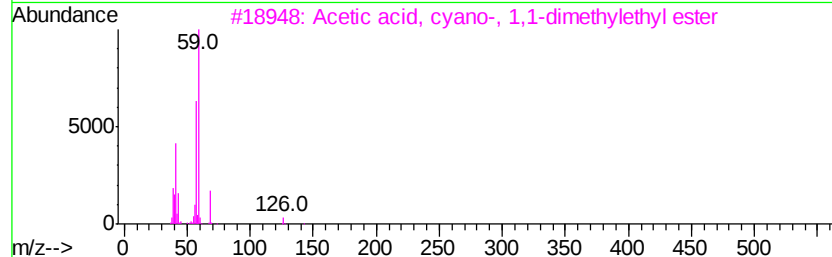
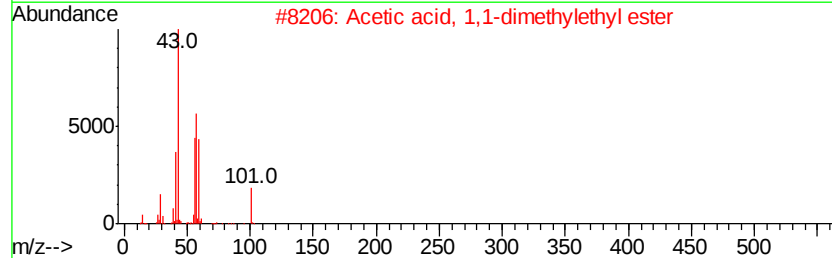
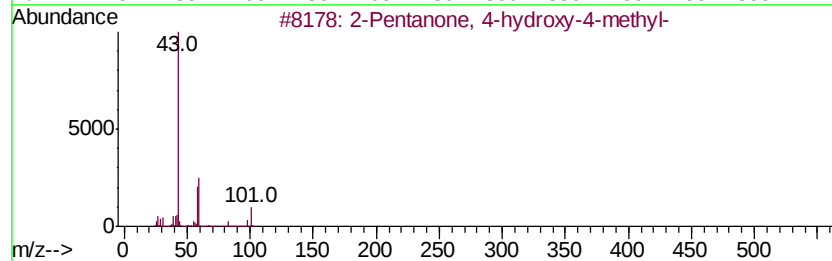
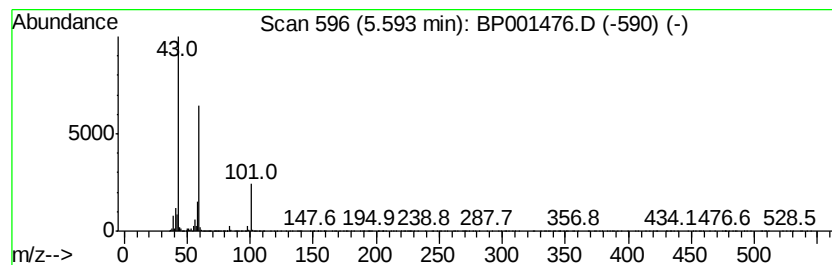
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.59	13.96 ng	97612	1,4-Dichlorobenzene-d4	8.28

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	38
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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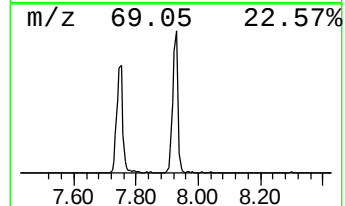
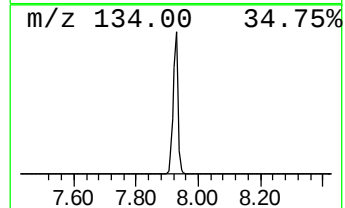
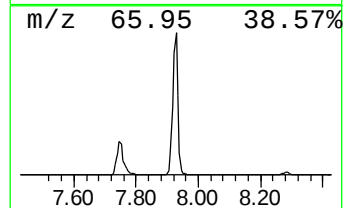
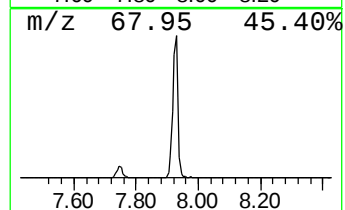
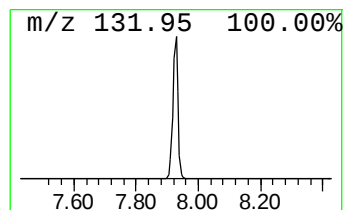
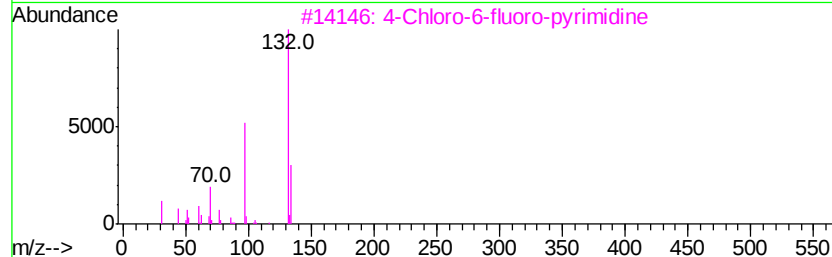
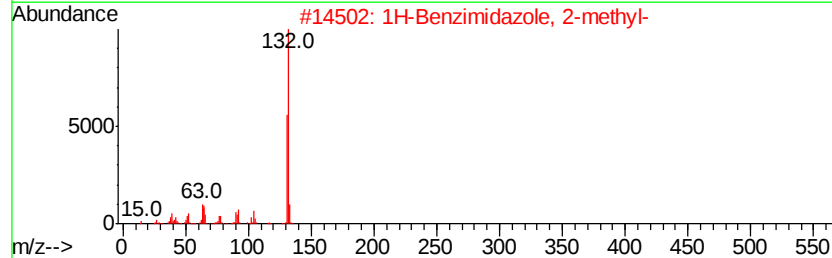
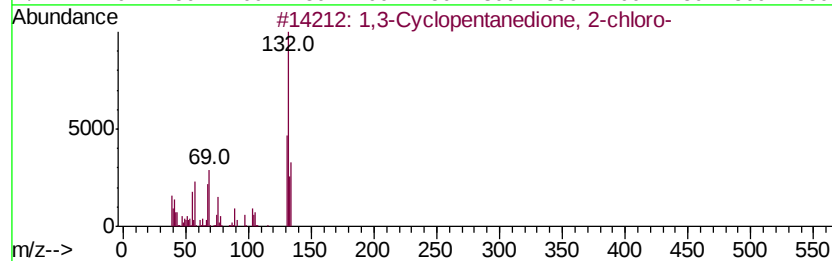
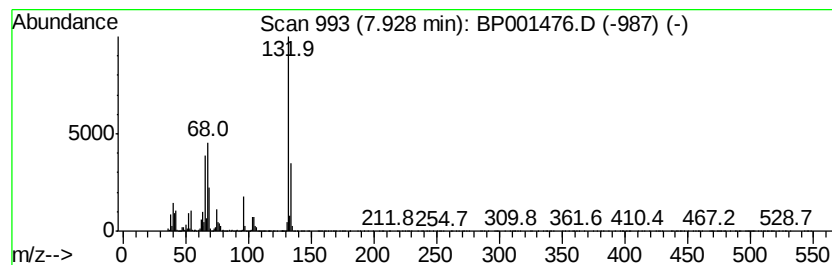
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown7.93 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	80.32 ng	561432	1,4-Dichlorobenzene-d4	8.28

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	22
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	10



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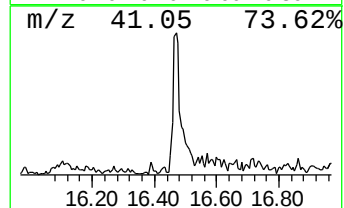
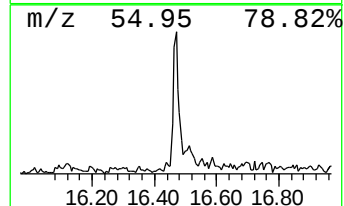
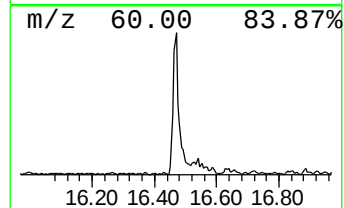
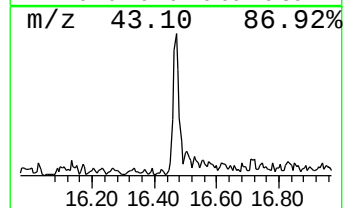
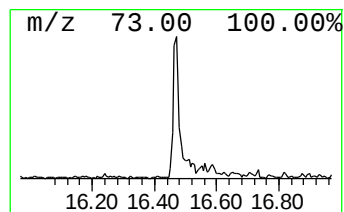
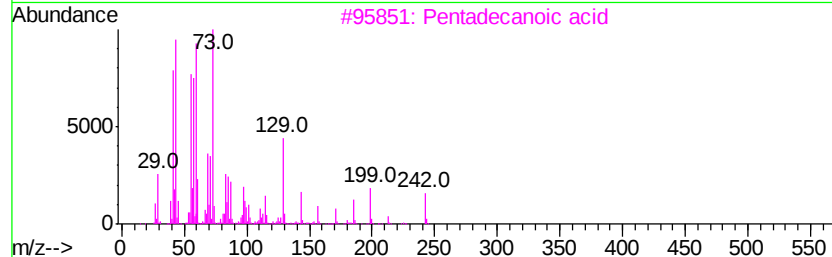
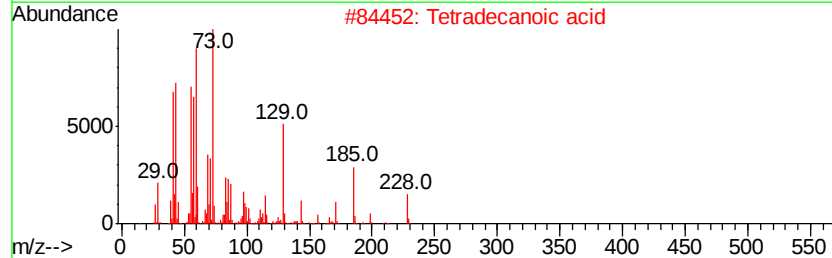
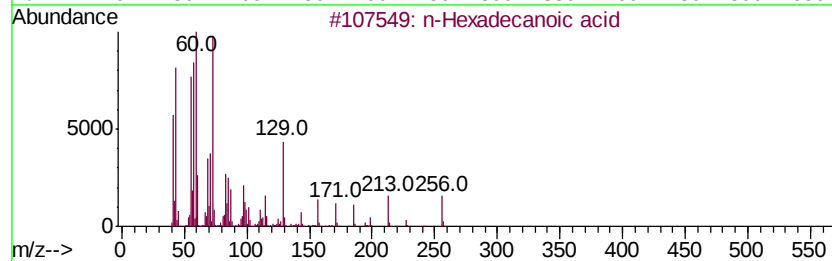
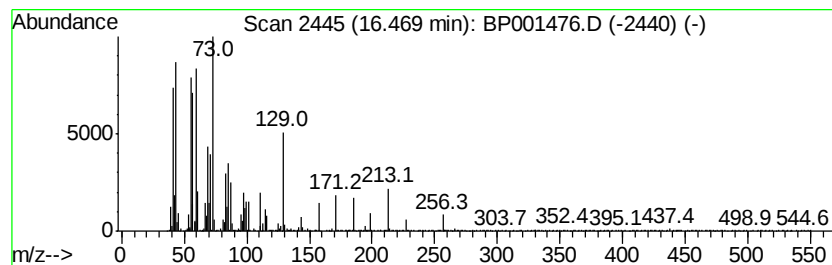
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.47	3.03 ng	33703	Phenanthrene-d10	15.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Tridecanoic acid	214	C13H26O2	000638-53-9	81
5		Octadecanoic acid	284	C18H36O2	000057-11-4	64



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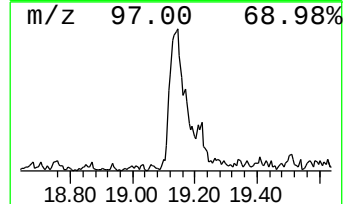
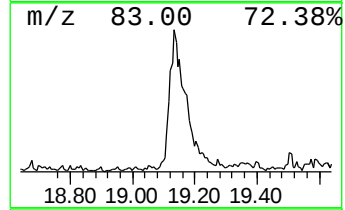
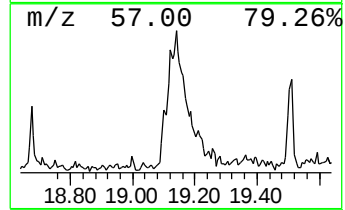
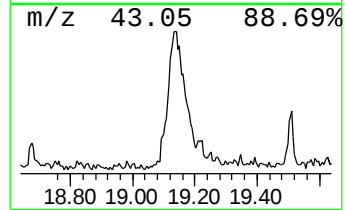
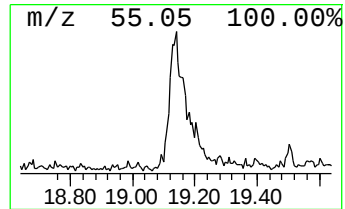
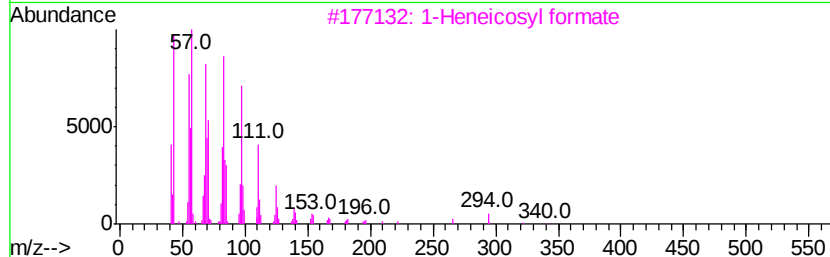
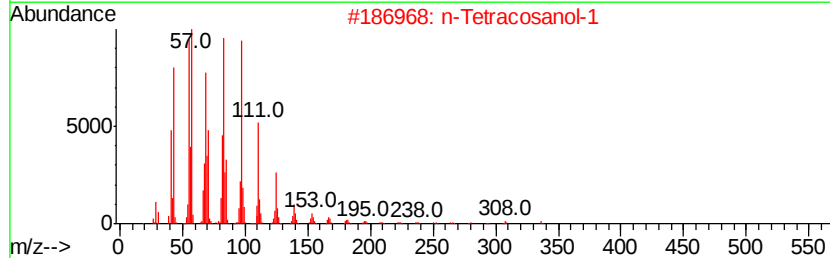
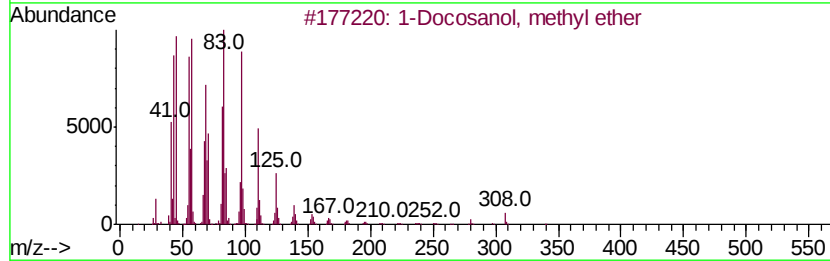
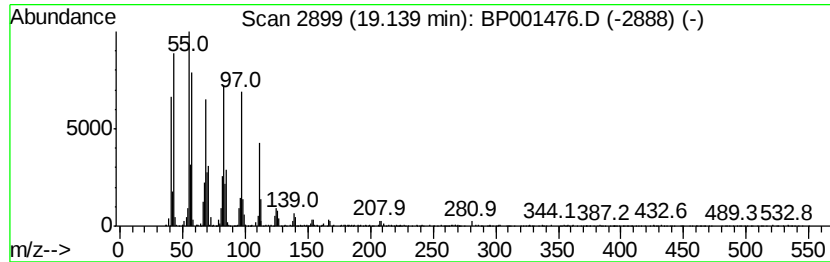
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Docosanol, methyl ether Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.14	8.31 ng	97775	Chrysene-d12	19.22

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosanol, methyl ether	340	C23H48O	1000333-91-9	93
2		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
3		1-Heneicosyl formate	340	C22H44O2	077899-03-7	90
4		9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	87



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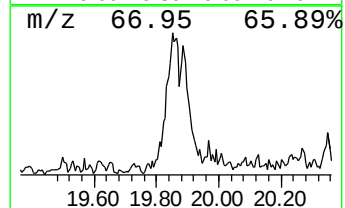
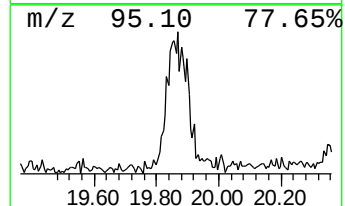
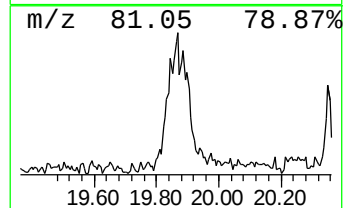
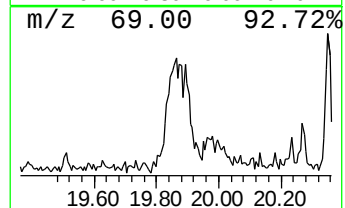
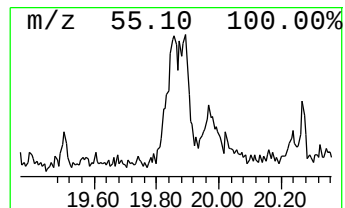
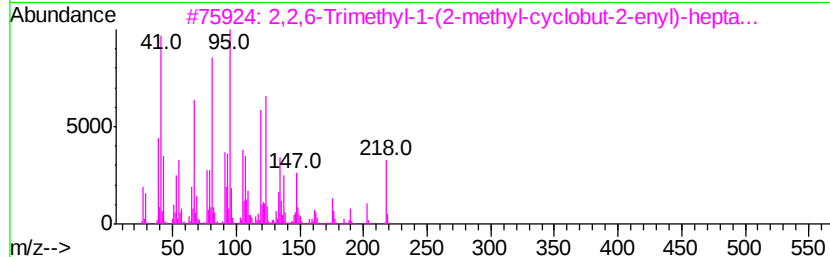
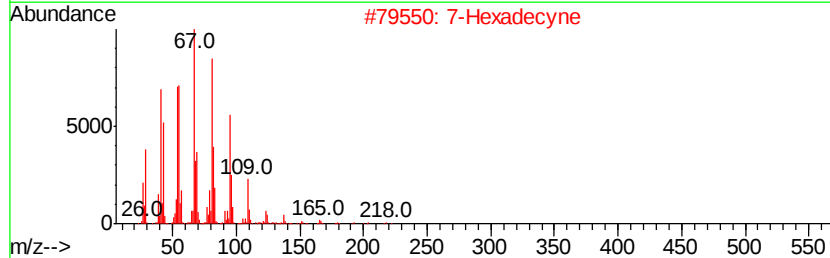
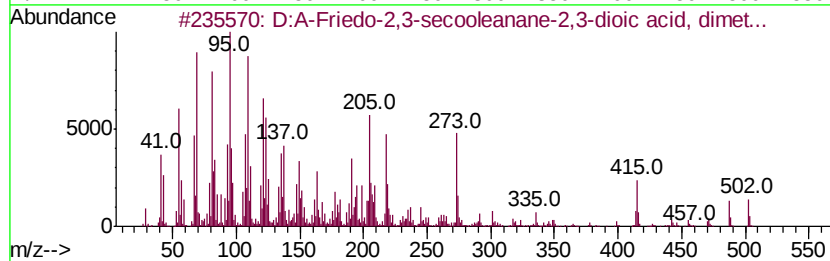
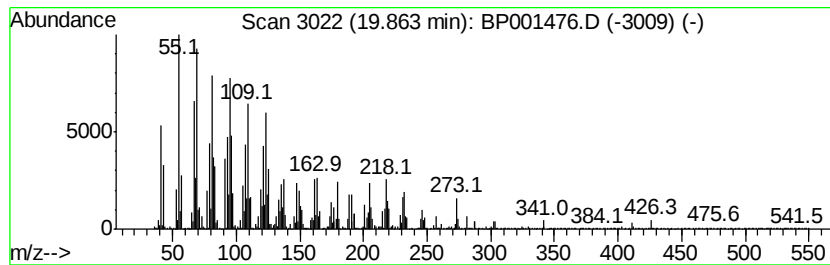
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 D:A-Friedo-2,3-secooleanane... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.86	9.22 ng	108454	Chrysene-d12	19.22	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:A-Friedo-2,3-secooleanane-2,3-...	502	C32H54O4	088373-58-4	93
2	7-Hexadecyne	222	C16H30	074685-28-2	70
3	2,2,6-Trimethyl-1-(2-methyl-cycl...	218	C15H22O	1000188-72-8	64
4	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	59
5	6-epi-shyobunol	222	C15H26O	1000374-18-3	51



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.59	14.0	ng	97612	1	8.28	139796	20.0
unknown7.93	7.93	80.3	ng	561432	1	8.28	139796	20.0
n-Hexadecanoic acid	16.47	3.0	ng	33703	4	15.57	222568	20.0
1-Docosanol, meth...	19.14	8.3	ng	97775	5	19.22	235260	20.0
D:A-Friedo-2,3-se...	19.86	9.2	ng	108454	5	19.22	235260	20.0