

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110222\
 Data File : BF130933.D
 Acq On : 02 Nov 2022 16:29
 Operator : CG\JU
 Sample : PB148741BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB148741BL

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-BF102722.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130933.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.281	23	33	38	rVB	98125	142384	4.79%	0.771%
2	2.387	46	51	59	rVB	43044	56500	1.90%	0.306%
3	5.163	517	523	534	rBV	266968	348290	11.72%	1.886%
4	5.545	583	588	591	rBV	2113539	2276412	76.59%	12.330%
5	6.545	752	758	761	rBV	2191940	2311547	77.77%	12.520%
6	6.922	818	822	825	rBV	644223	501112	16.86%	2.714%
7	7.486	912	918	921	rBV	1523963	1526688	51.37%	8.269%
8	8.210	1036	1041	1044	rBV	641925	653137	21.98%	3.538%
9	9.286	1218	1224	1227	rBV	3035819	2754244	92.67%	14.918%
10	9.969	1335	1340	1343	rBV	935857	765353	25.75%	4.145%
11	10.763	1470	1475	1478	rBV	2152624	1853507	62.36%	10.039%
12	11.463	1590	1594	1597	rBV	1021450	811482	27.30%	4.395%
13	13.057	1860	1865	1868	rBV	3275632	2972143	100.00%	16.098%
14	14.110	2040	2044	2048	rBV	715006	624319	21.01%	3.381%
15	14.327	2073	2081	2095	rVB5	15509	59683	2.01%	0.323%
16	15.621	2296	2301	2310	rBV	343373	487230	16.39%	2.639%
17	16.109	2380	2384	2389	rVB2	25530	37716	1.27%	0.204%
18	16.651	2471	2476	2482	rVB4	25362	46184	1.55%	0.250%
19	17.280	2579	2583	2597	rVB3	23115	70309	2.37%	0.381%
20	17.574	2627	2633	2650	rVB6	26135	119572	4.02%	0.648%
21	18.027	2706	2710	2719	rVB5	17794	45079	1.52%	0.244%

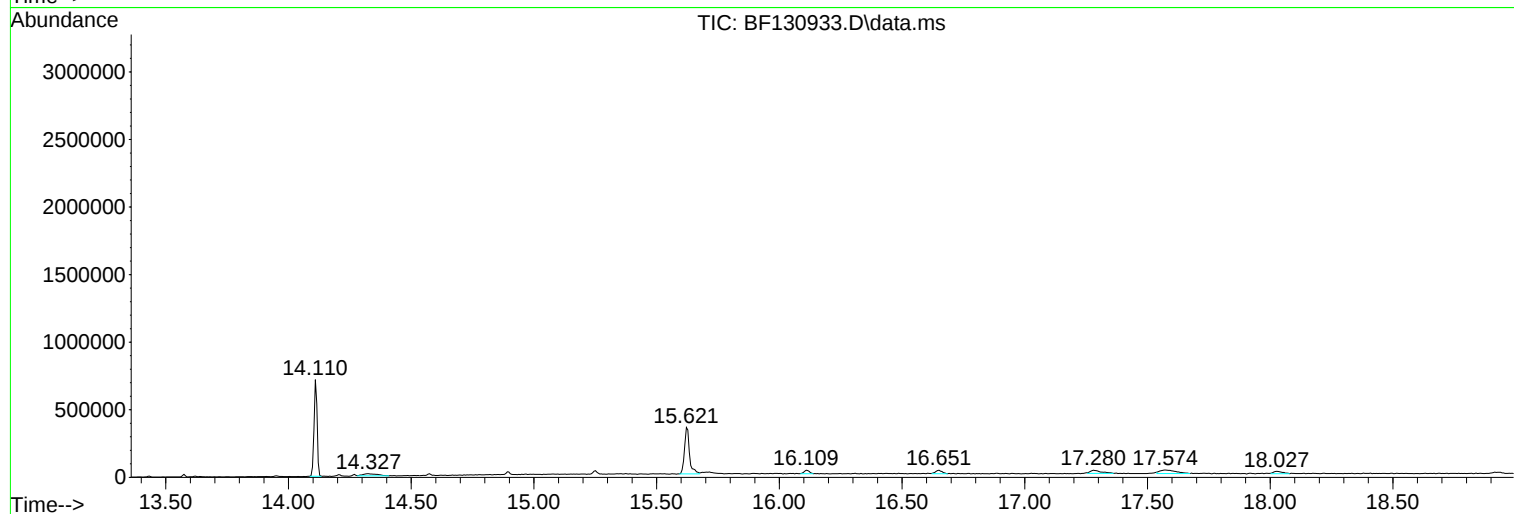
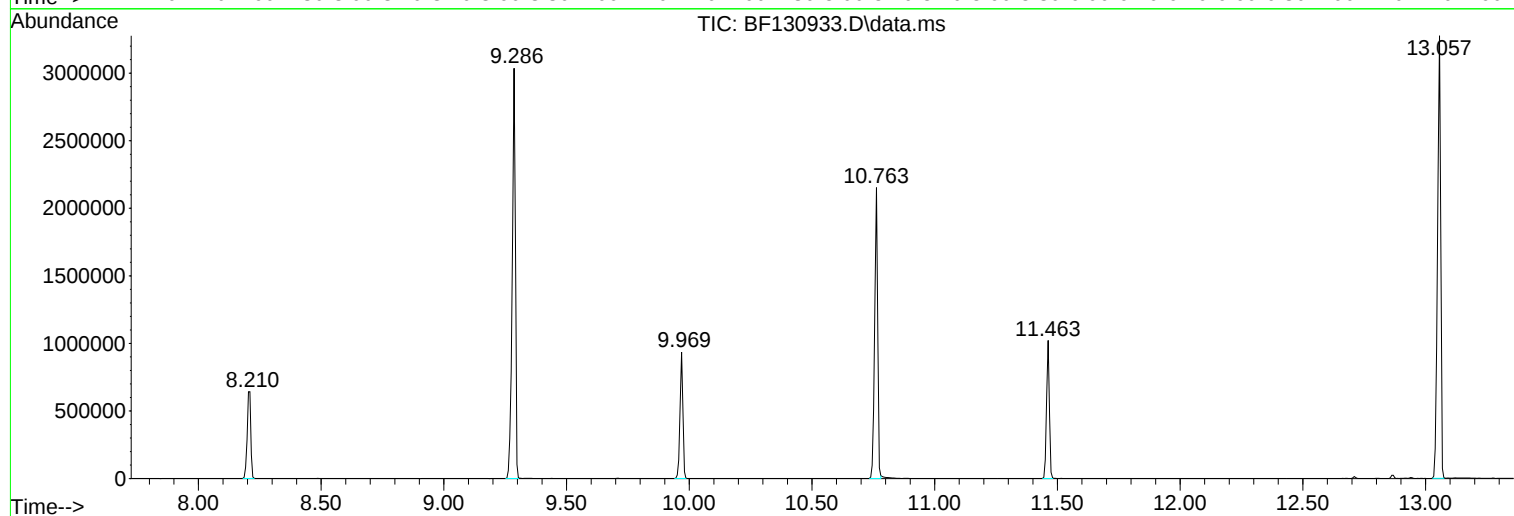
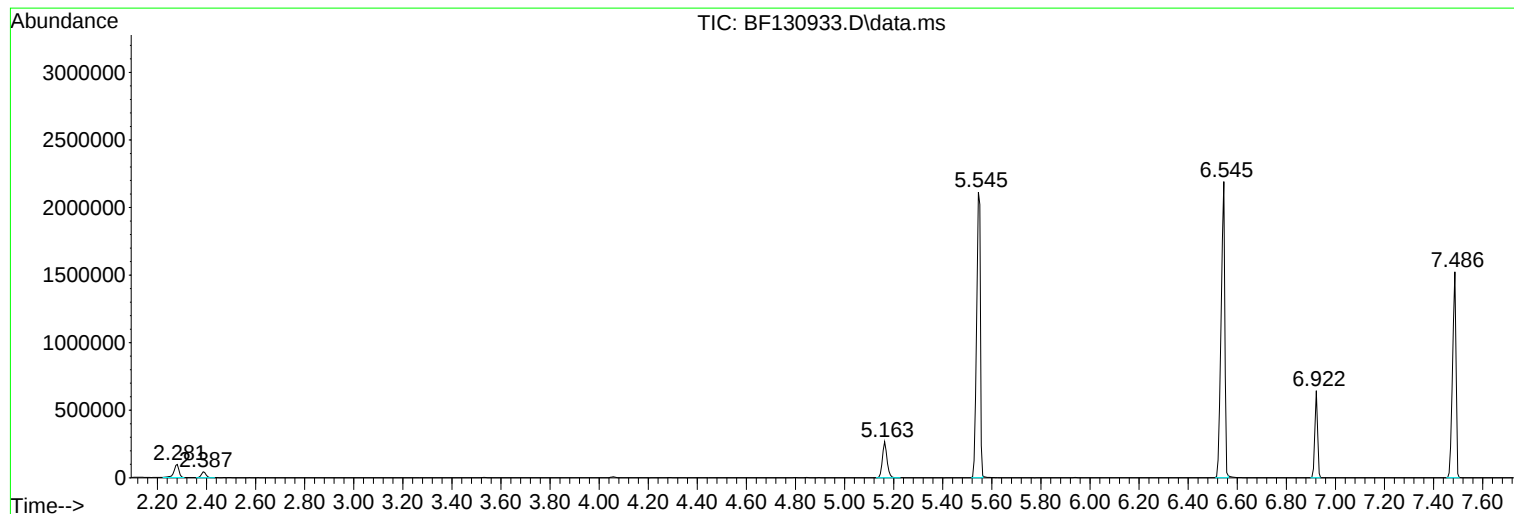
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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ClientSampleId :
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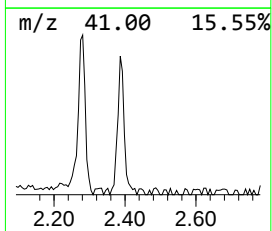
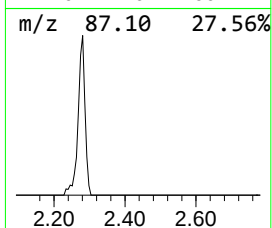
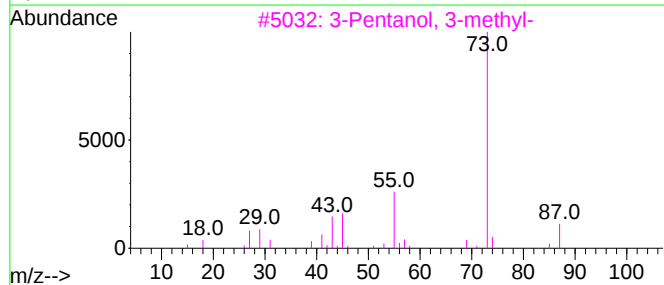
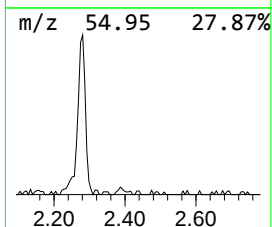
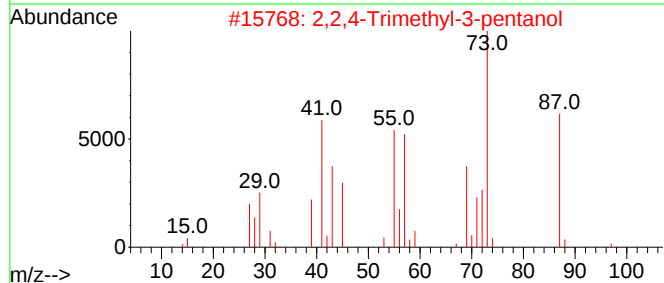
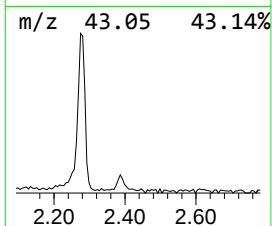
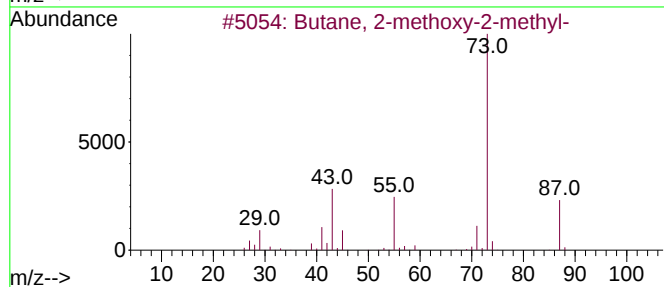
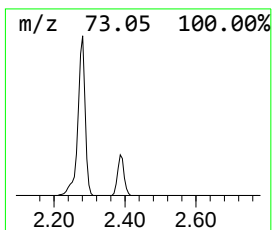
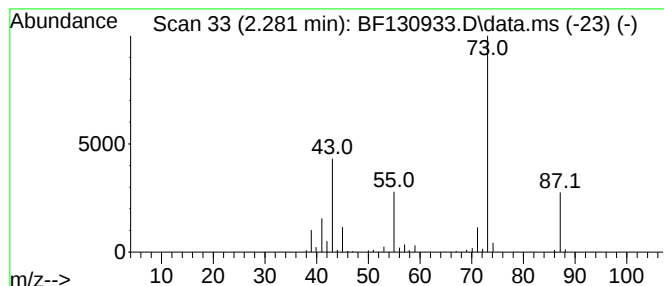
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF102722.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.281	5.68 ng	142384	1,4-Dichlorobenzene-d4	6.922

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		3-Pentanol, 3-methyl-	102	C6H14O	000077-74-7	38
4		Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5		1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	23



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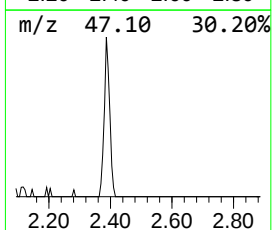
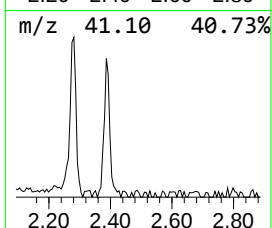
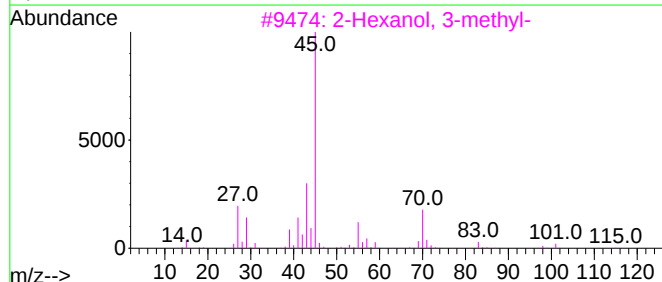
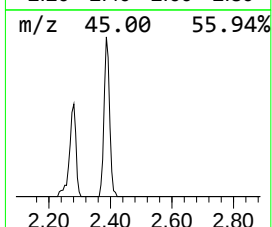
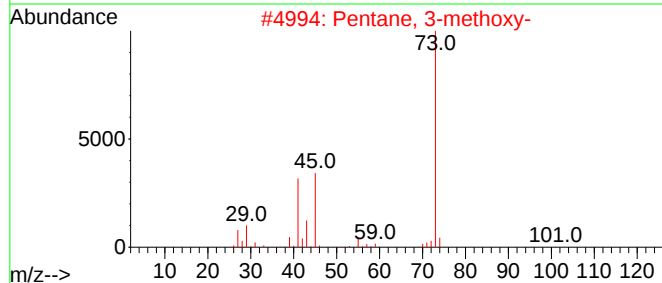
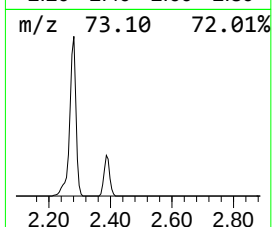
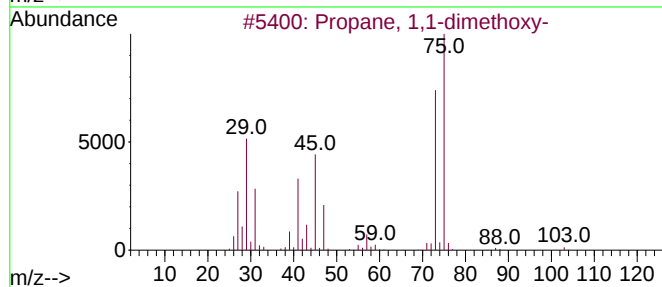
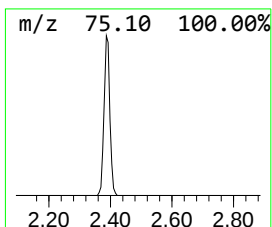
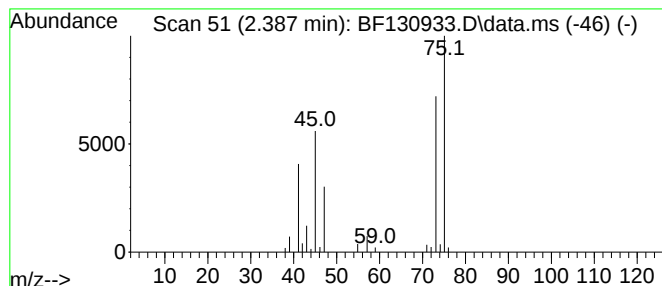
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propane, 1,1-dimethoxy- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.387	2.25 ng	56500	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	74
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	22
3			2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	9
4			2-Pentanol	88	C5H12O	006032-29-7	9
5			Acetic acid, methoxy-, methyl ester	104	C4H8O3	006290-49-9	9



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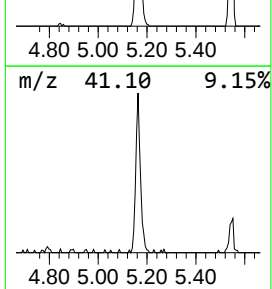
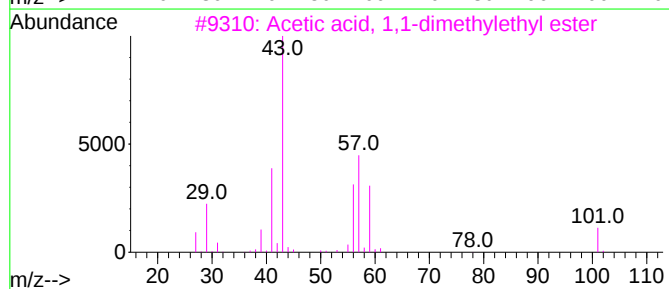
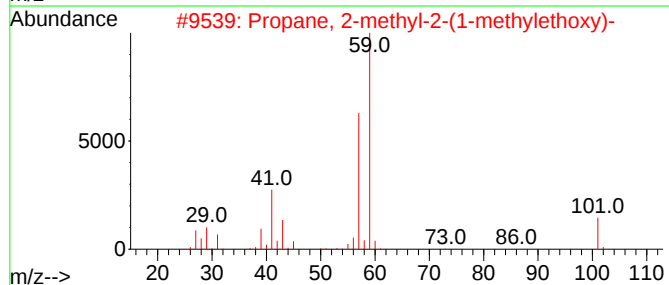
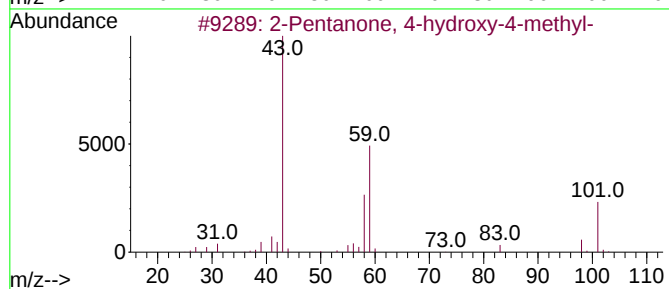
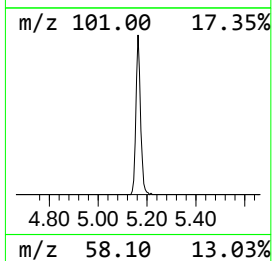
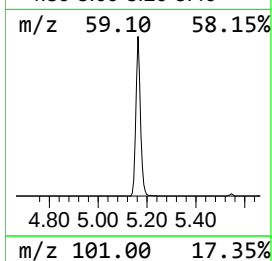
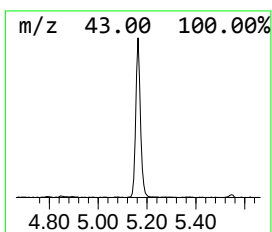
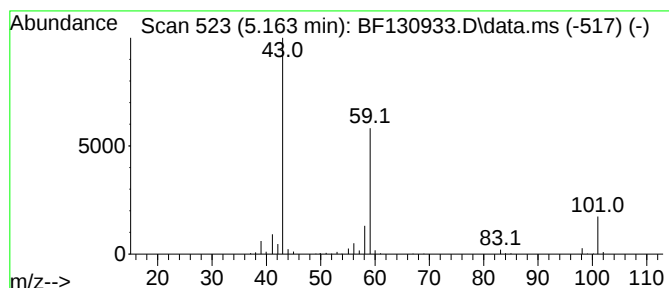
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.163	13.90 ng	348290	1,4-Dichlorobenzene-d4	6.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	23



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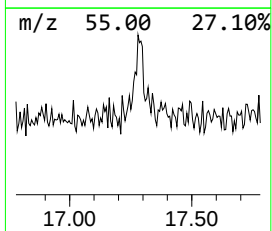
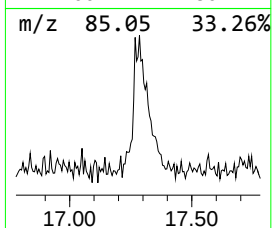
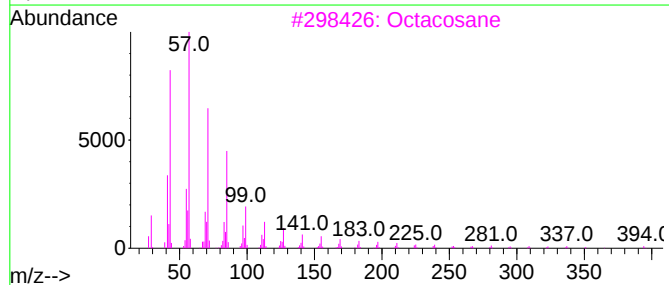
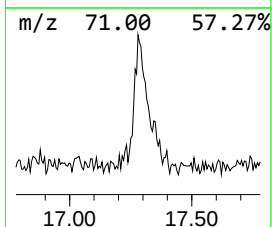
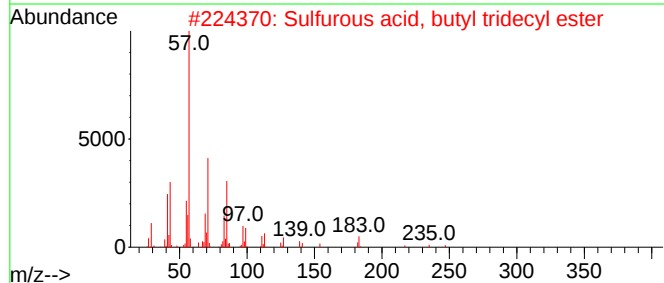
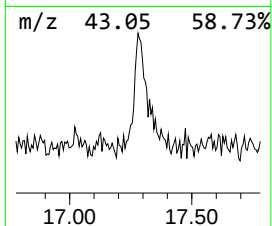
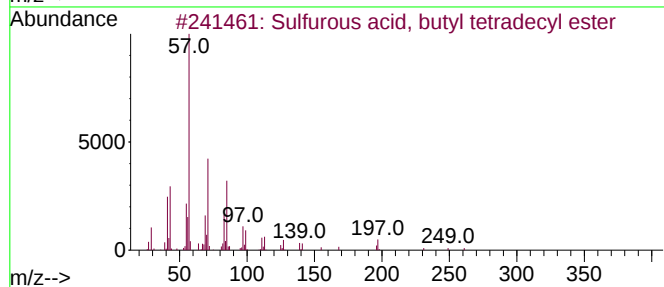
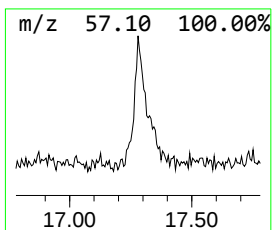
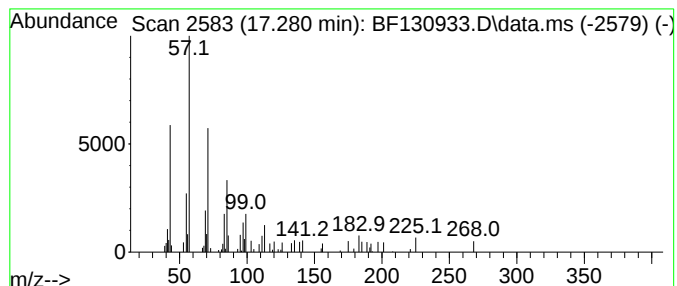
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Peak Number 4 Sulfurous acid, butyl tetra... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.280	2.89 ng	70309	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1010309-18-1	80
2			Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	72
3			Octacosane	394	C28H58	000630-02-4	72
4			Sulfurous acid, butyl pentadecyl...	348	C19H40O3S	1000309-18-2	72
5			Hentriacontane	437	C31H64	000630-04-6	72



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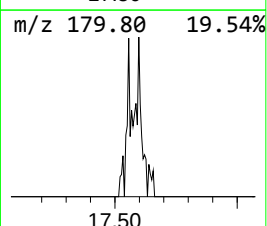
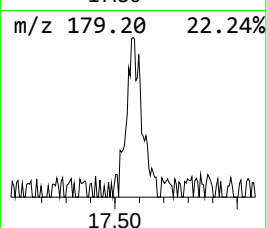
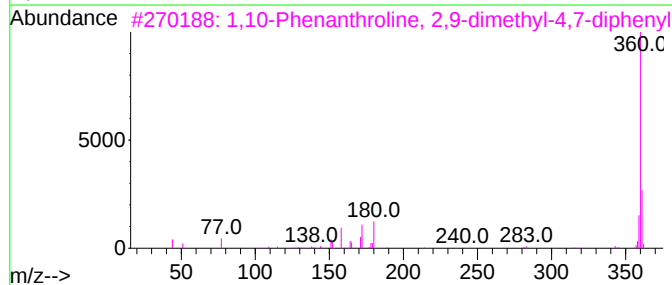
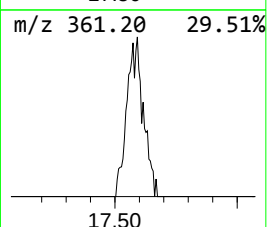
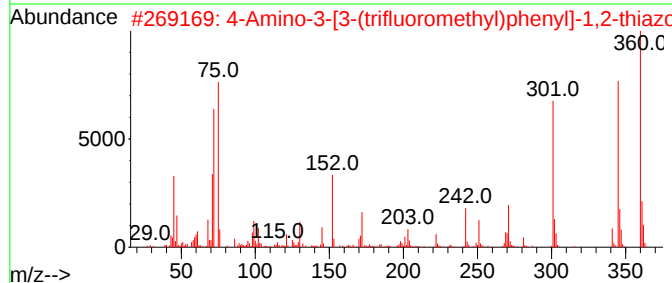
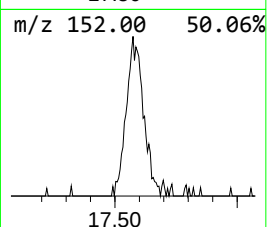
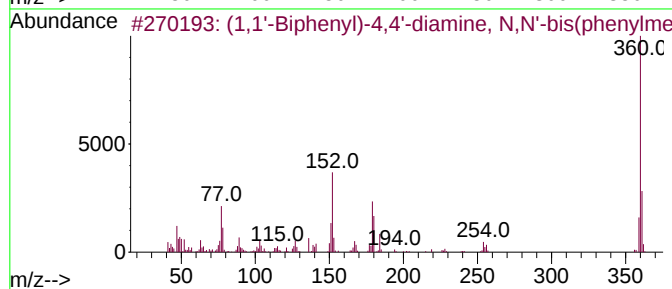
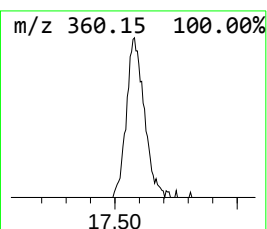
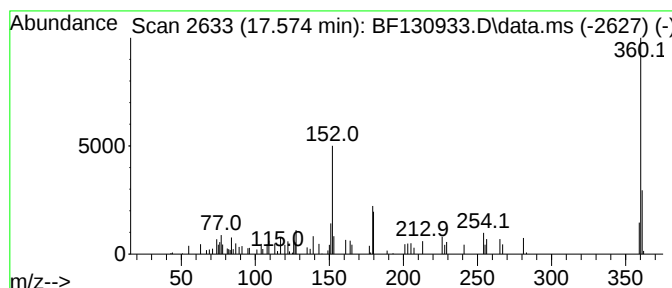
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TIC Integration Parameters: LSCINT.P

Peak Number 5 (1,1'-Biphenyl)-4,4'-diamin... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.574	4.91 ng	119572	Perylene-d12	15.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			(1,1'-Biphenyl)-4,4'-diamine, N,...	360	C26H20N2	006311-48-4	87
2			4-Amino-3-[3-(trifluoromethyl)ph...	360	C14H15F3N2O2SSi	1010500-98-0	50
3			1,10-Phenanthroline, 2,9-dimethy...	360	C26H20N2	004733-39-5	47
4			N,N'-di-2-Naphthyl-p-phenylenedi...	360	C26H20N2	000093-46-9	37
5			2,6-Diiodo-p-benzoquinone	360	C6H2I2O2	020389-01-9	35



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.281	5.7	ng	142384	1	6.922	501112	20.0
Propane, 1,1-di...	2.387	2.3	ng	56500	1	6.922	501112	20.0
2-Pentanone, 4-...	5.163	13.9	ng	348290	1	6.922	501112	20.0
Sulfurous acid,...	17.280	2.9	ng	70309	6	15.621	487230	20.0
(1,1'-Biphenyl)...	17.574	4.9	ng	119572	6	15.621	487230	20.0