

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG040124\
 Data File : BG060715.D
 Acq On : 1 Apr 2024 14:37
 Operator : MA/JU
 Sample : P1917-01
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 CCM-2

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-BG032924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG060715.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.100	13	19	27	rBV3	32384	60828	1.46%	0.303%
2	3.176	27	32	43	rVB	312450	441096	10.57%	2.197%
3	4.481	250	254	261	rBV	51917	74349	1.78%	0.370%
4	5.080	349	356	366	rBV	1138937	1683488	40.36%	8.387%
5	5.533	425	433	441	rBV	738602	1151837	27.61%	5.738%
6	7.107	692	701	709	rBV	852455	1408627	33.77%	7.017%
7	7.953	839	845	852	rBV	219244	366743	8.79%	1.827%
8	9.105	1032	1041	1051	rBV	431613	729854	17.50%	3.636%
9	10.527	1275	1283	1293	rBV	44211	77077	1.85%	0.384%
10	10.750	1312	1321	1328	rBV	321450	561550	13.46%	2.797%
11	13.212	1732	1740	1749	rVB	1355948	2101073	50.37%	10.467%
12	14.581	1964	1973	1981	rVB	580491	902283	21.63%	4.495%
13	14.810	2002	2012	2017	rBV4	26636	66752	1.60%	0.333%
14	16.067	2219	2226	2235	rBV	826756	1242919	29.80%	6.192%
15	17.330	2434	2441	2447	rBV	815047	1265007	30.32%	6.302%
16	18.241	2591	2596	2601	rBV2	43361	67216	1.61%	0.335%
17	19.957	2879	2888	2897	rBV	3117219	4171523	100.00%	20.781%
18	20.298	2942	2946	2951	rVB	38414	43820	1.05%	0.218%
19	20.791	3027	3030	3035	rVB	52618	58788	1.41%	0.293%
20	21.296	3110	3116	3128	rVB2	101756	221008	5.30%	1.101%
21	21.590	3159	3166	3178	rVB	830427	1415738	33.94%	7.053%
22	21.849	3206	3210	3216	rVB	63024	92919	2.23%	0.463%
23	22.460	3309	3314	3319	rBV2	62552	96313	2.31%	0.480%
24	23.153	3427	3432	3436	rBV	41374	68265	1.64%	0.340%
25	23.335	3458	3463	3473	rVB	58909	118945	2.85%	0.593%
26	23.964	3566	3570	3578	rVB3	38221	80951	1.94%	0.403%
27	24.722	3690	3699	3713	rVB	527890	1504491	36.07%	7.495%

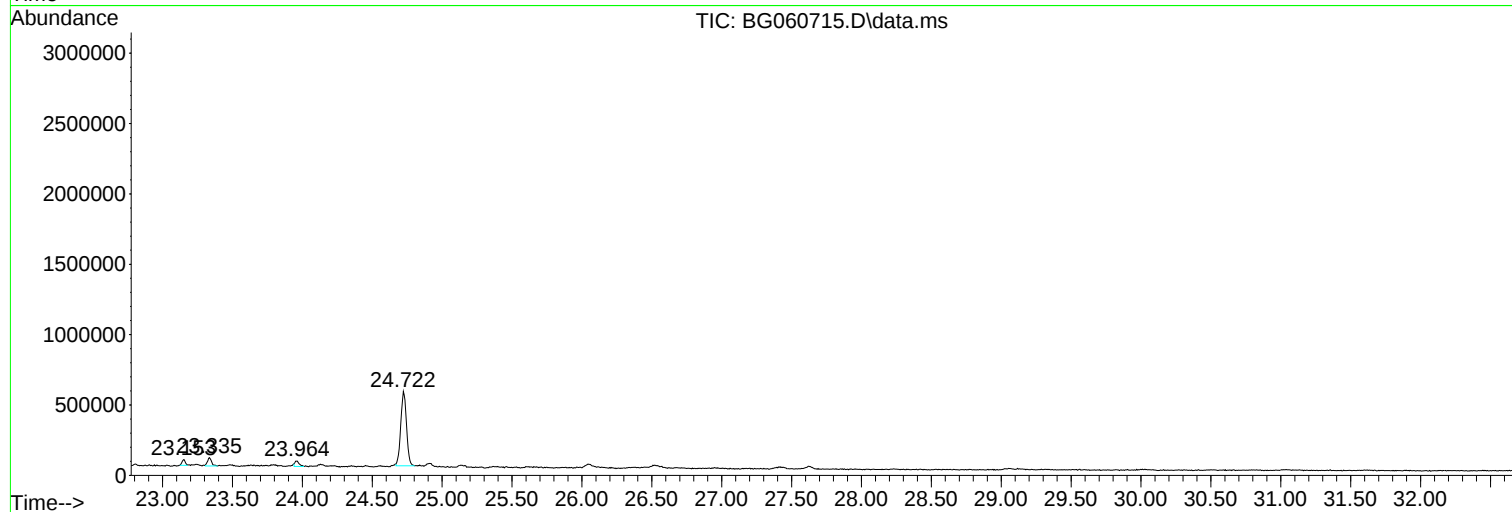
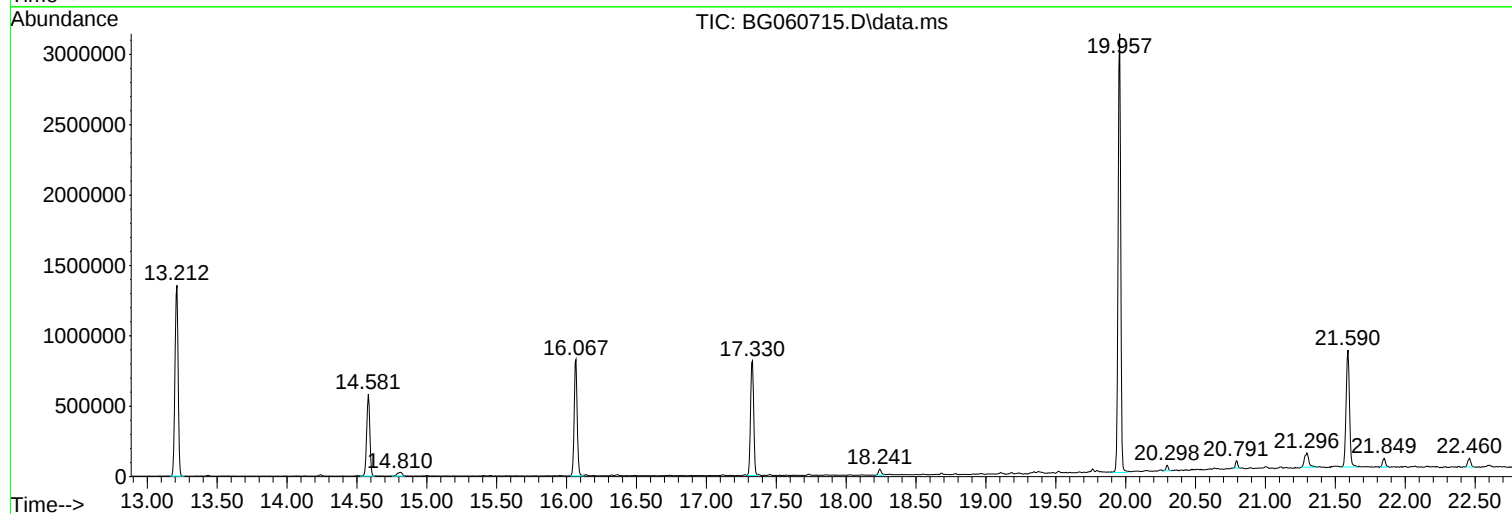
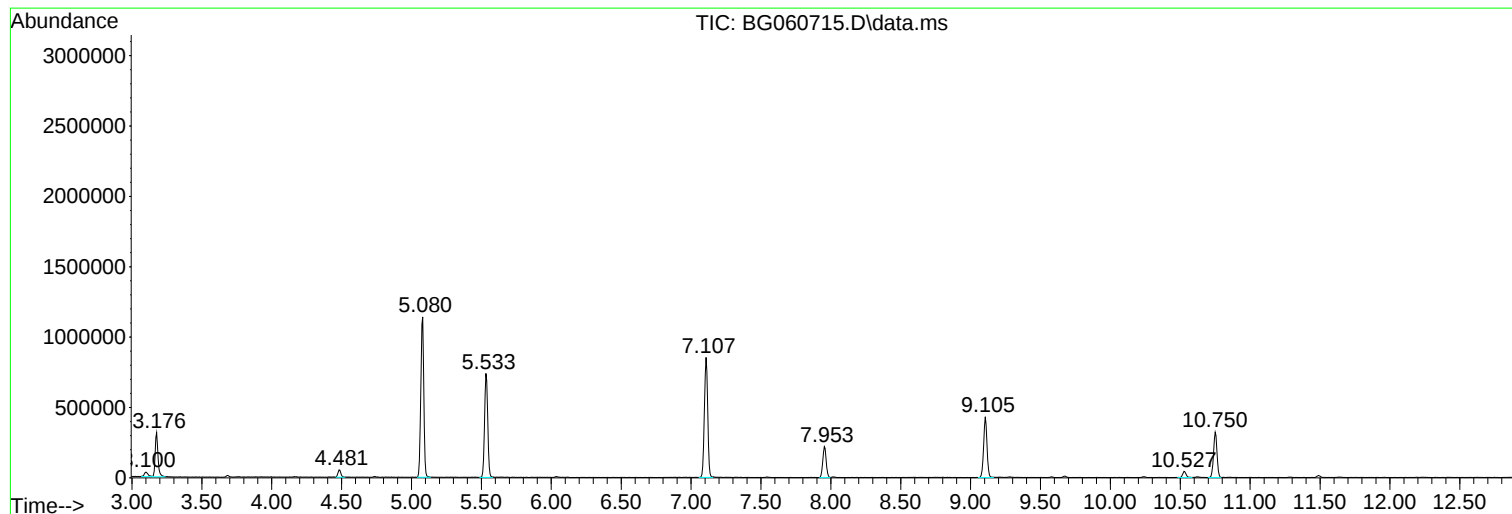
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Instrument :
BNA_G
ClientSampleId :
CCM-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG032924.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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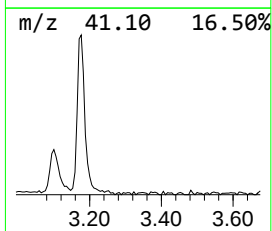
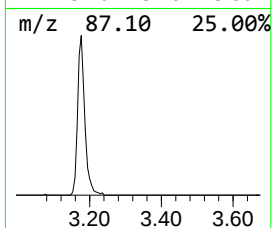
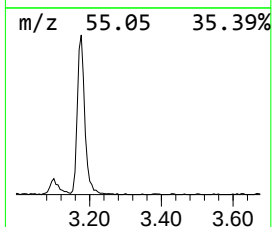
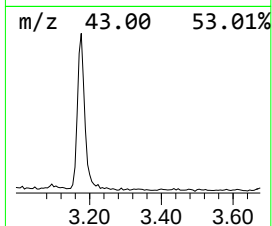
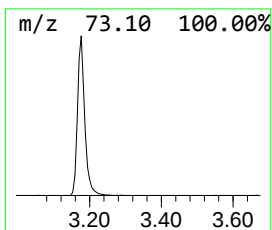
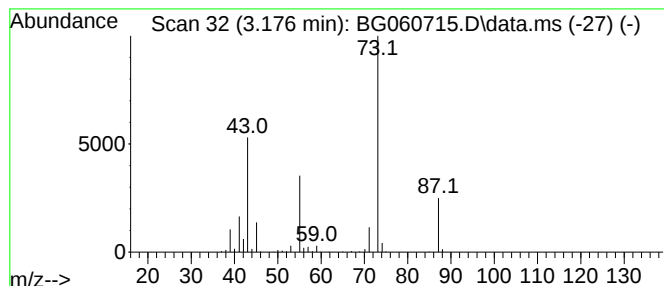
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.176	24.05 ng	441096	1,4-Dichlorobenzene-d4	7.953

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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	17
5			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



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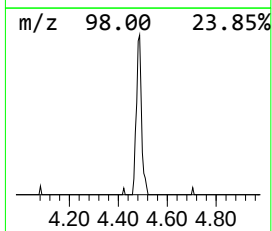
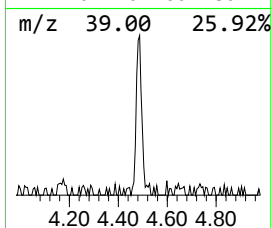
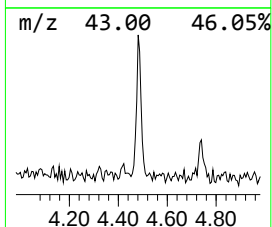
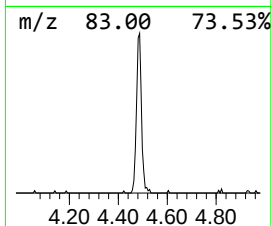
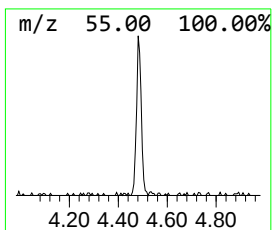
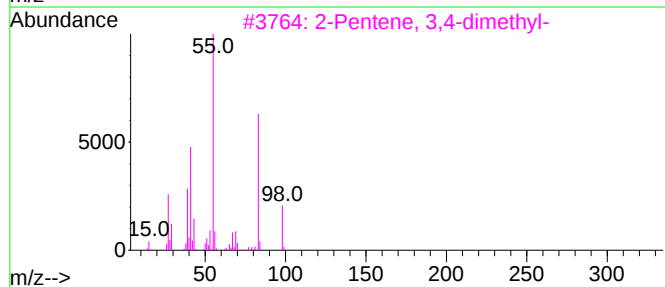
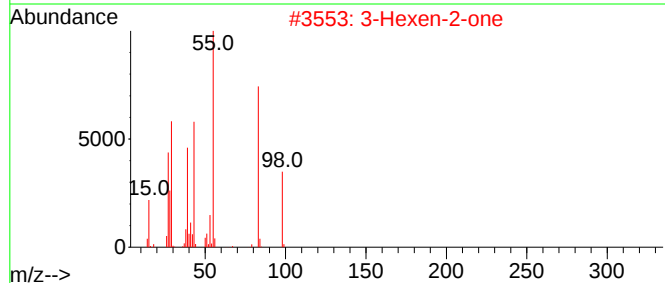
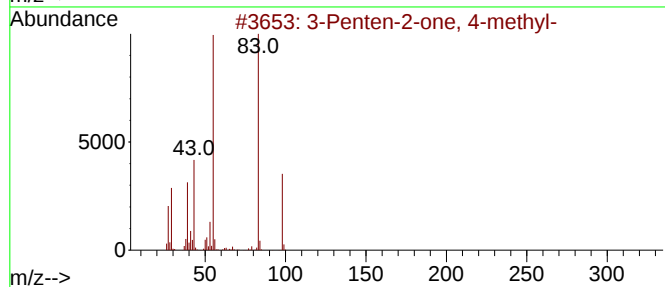
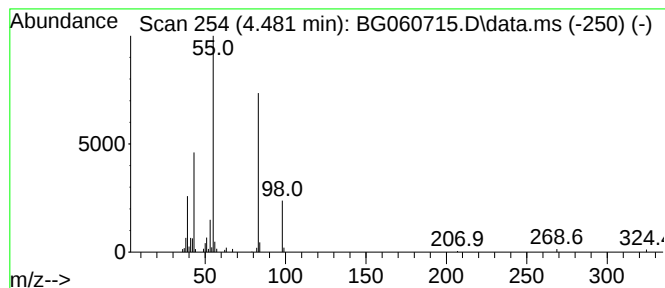
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TIC Integration Parameters: LSCINT.P

Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	4.05 ng	74349	1,4-Dichlorobenzene-d4	7.953

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	90
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-	98	C7H14	024910-63-2	86
4		2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86
5		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86



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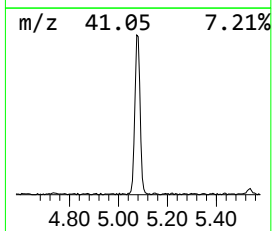
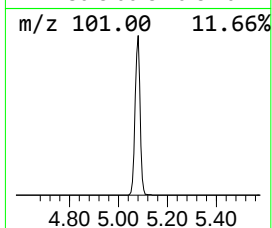
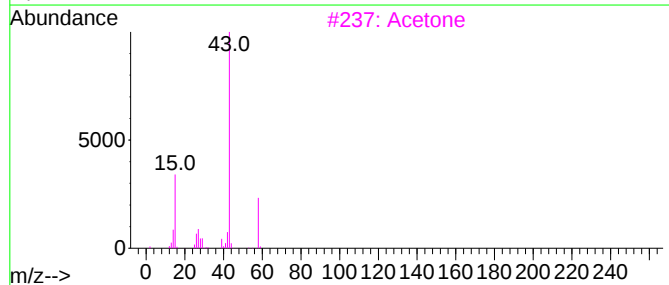
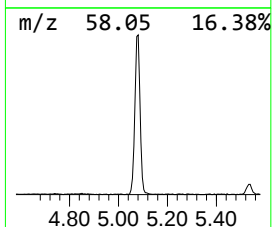
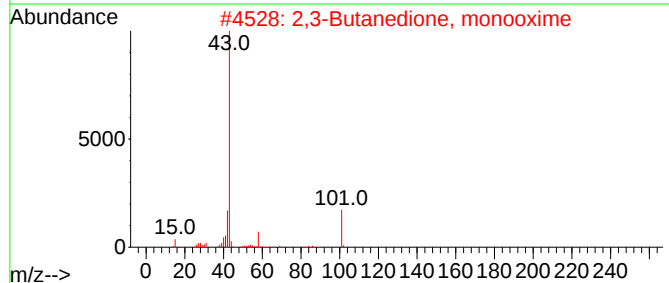
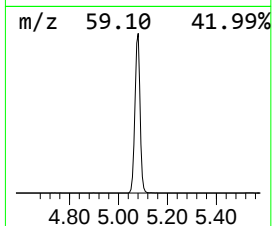
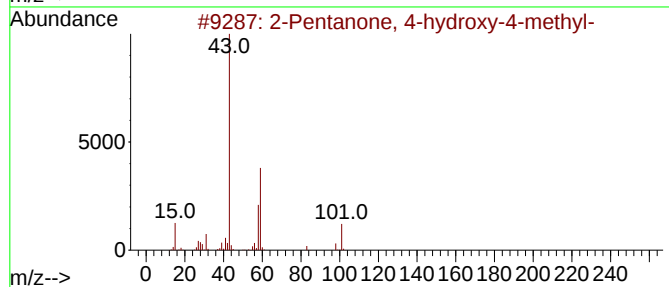
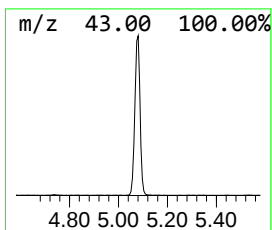
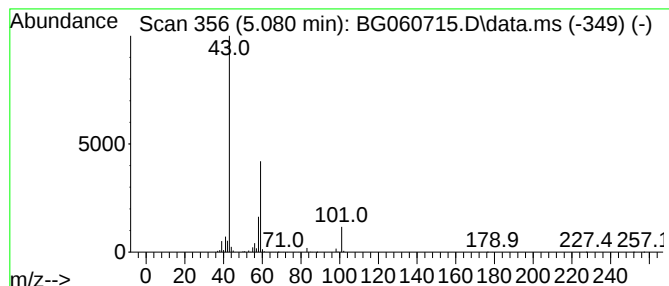
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.080	91.81 ng	1683490	1,4-Dichlorobenzene-d4	7.953

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	83
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3			Acetone	58	C3H6O	000067-64-1	12
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5			5-Aminovaleric acid	117	C5H11NO2	000660-88-8	9



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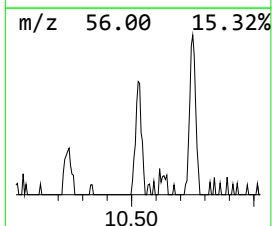
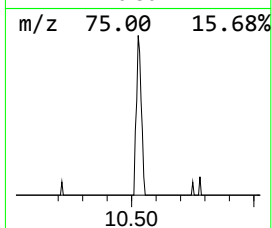
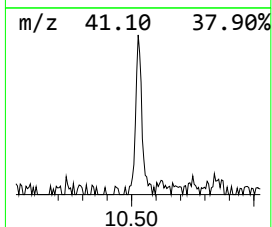
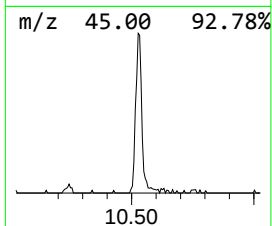
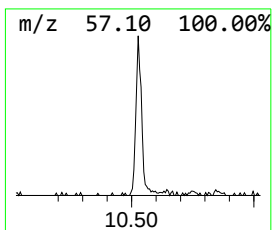
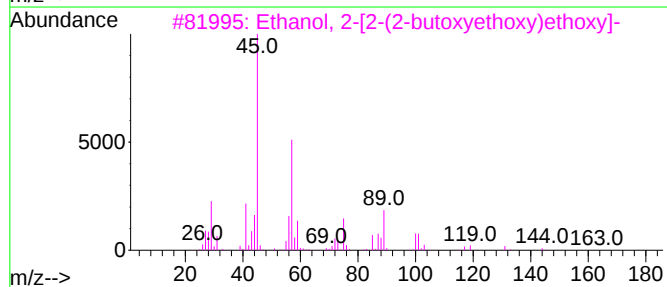
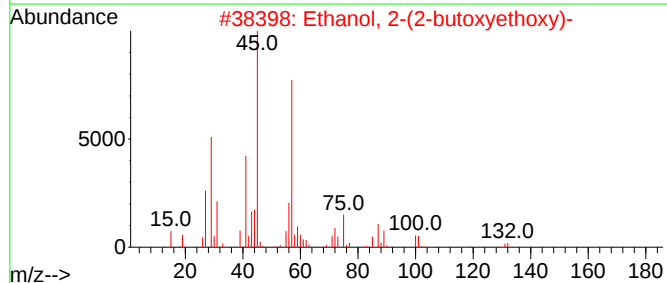
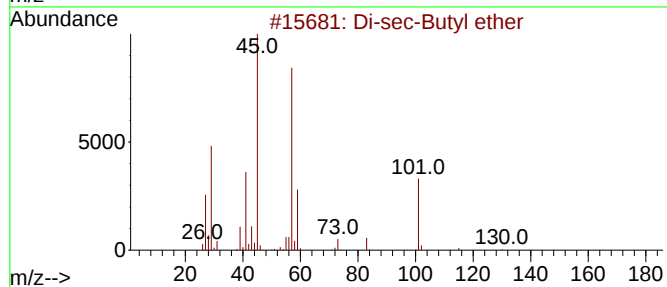
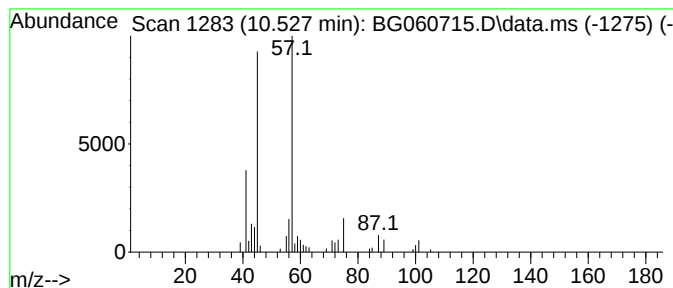
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Di-sec-Butyl ether Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.527	2.75 ng	77077	Naphthalene-d8	10.750

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	59
2			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	56
3			Ethanol, 2-[2-(2-butoxyethoxy)et...	206	C10H22O4	000143-22-6	50
4			Propanoic acid, 2-(methoxymethoxy)-	134	C5H10O4	081327-29-9	50
5			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50



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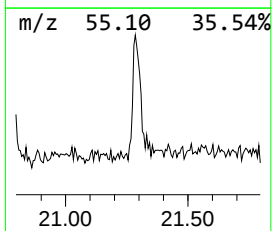
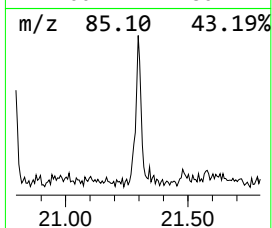
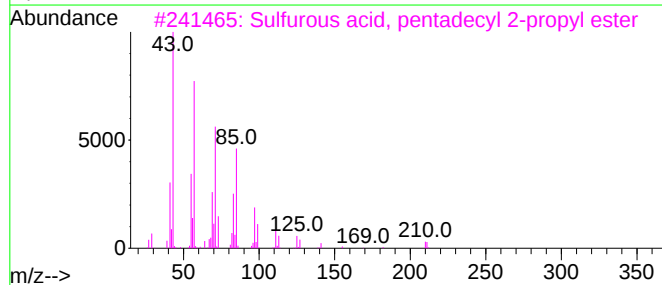
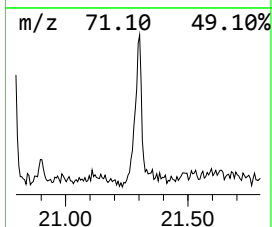
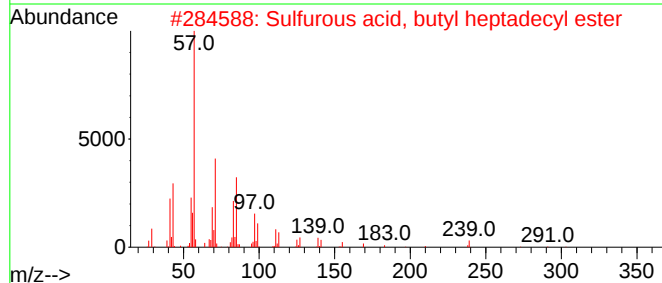
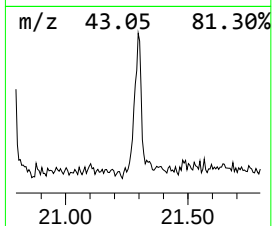
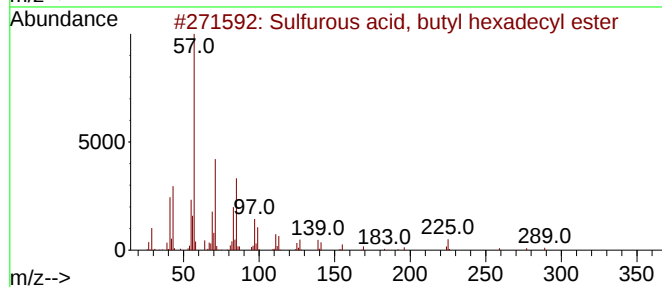
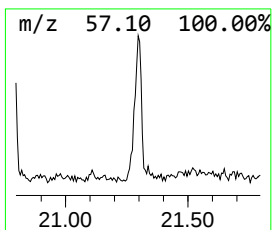
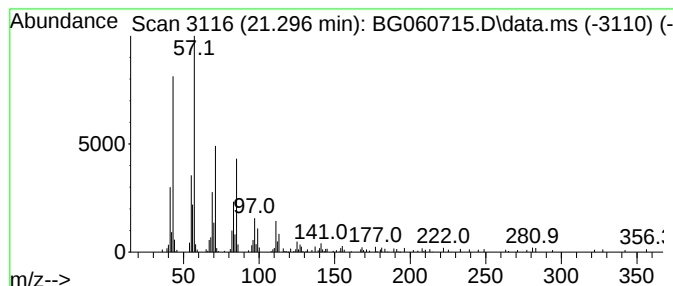
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TIC Library : C:\Database\NIST20.L
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Peak Number 6 Sulfurous acid, butyl hexad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.296	3.12 ng	221008	Chrysene-d12	21.590

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, butyl hexadecyl ...	362	C20H42O3S	1000309-18-3	91
2			Sulfurous acid, butyl heptadecyl...	376	C21H44O3S	1000309-18-4	91
3			Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	83
4			Heptacosane, 1-chloro-	414	C27H55Cl	062016-79-9	80
5			Sulfurous acid, butyl octadecyl ...	390	C22H46O3S	1000309-18-5	80



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.176	24.1	ng	441096	1	7.953	366743	20.0
3-Penten-2-one,...	4.481	4.0	ng	74349	1	7.953	366743	20.0
2-Pentanone, 4-...	5.080	91.8	ng	1683490	1	7.953	366743	20.0
Di-sec-Butyl ether	10.527	2.8	ng	77077	2	10.750	561550	20.0
Sulfurous acid,...	21.296	3.1	ng	221008	5	21.590	1415740	20.0