

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG121622\
 Data File : BG055996.D
 Acq On : 16 Dec 2022 16:24
 Operator : CG/JU
 Sample : N6037-17
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RB-25-(7-9)

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-BG121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG055996.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.400	15	19	30	rBB	24931	38115	4.78%	1.136%
2	5.415	357	362	367	rBB	13196	18686	2.34%	0.557%
3	5.891	436	443	449	rBB	103926	167459	21.01%	4.990%
4	7.501	710	717	724	rBB	107897	183529	23.02%	5.468%
5	8.371	860	865	871	rBB	24713	40123	5.03%	1.195%
6	9.546	1058	1065	1071	rBB	63177	111230	13.95%	3.314%
7	11.209	1341	1348	1354	rBB	32271	55866	7.01%	1.665%
8	13.612	1750	1757	1763	rBB	226866	355338	44.58%	10.588%
9	14.981	1984	1990	1996	rBV	63930	97159	12.19%	2.895%
10	16.455	2235	2241	2252	rVB	327244	491672	61.68%	14.650%
11	16.637	2257	2272	2277	rBB	14675	27788	3.49%	0.828%
12	17.719	2449	2456	2461	rBV	107823	160263	20.11%	4.775%
13	17.754	2461	2462	2468	rVB2	7237	8415	1.06%	0.251%
14	18.565	2595	2600	2607	rBV3	32141	46892	5.88%	1.397%
15	19.746	2796	2801	2806	rVB	22903	32674	4.10%	0.974%
16	19.816	2809	2813	2820	rVV4	8023	12270	1.54%	0.366%
17	20.104	2850	2862	2868	rBV	31414	51198	6.42%	1.525%
18	20.292	2888	2894	2899	rBV	624491	797113	100.00%	23.751%
19	20.568	2934	2941	2942	rBV6	5995	11347	1.42%	0.338%
20	20.750	2965	2972	2975	rBV3	8001	13687	1.72%	0.408%
21	20.885	2993	2995	3001	rVB4	7294	10967	1.38%	0.327%
22	21.614	3115	3119	3124	rVB3	18662	27375	3.43%	0.816%
23	22.025	3180	3189	3194	rBV2	116883	232542	29.17%	6.929%
24	22.078	3194	3198	3205	rVB	19224	36687	4.60%	1.093%
25	22.883	3332	3335	3341	rVB5	6923	13393	1.68%	0.399%
26	23.835	3493	3497	3503	rVB9	7269	12057	1.51%	0.359%
27	24.405	3587	3594	3598	rBV4	12849	35395	4.44%	1.055%
28	25.186	3723	3727	3728	rBV4	7900	10559	1.32%	0.315%
29	25.357	3747	3756	3767	rVB2	15990	47053	5.90%	1.402%
30	25.527	3775	3785	3793	rBV2	63626	197215	24.74%	5.876%
31	29.528	4458	4466	4467	rBV7	6000	12123	1.52%	0.361%

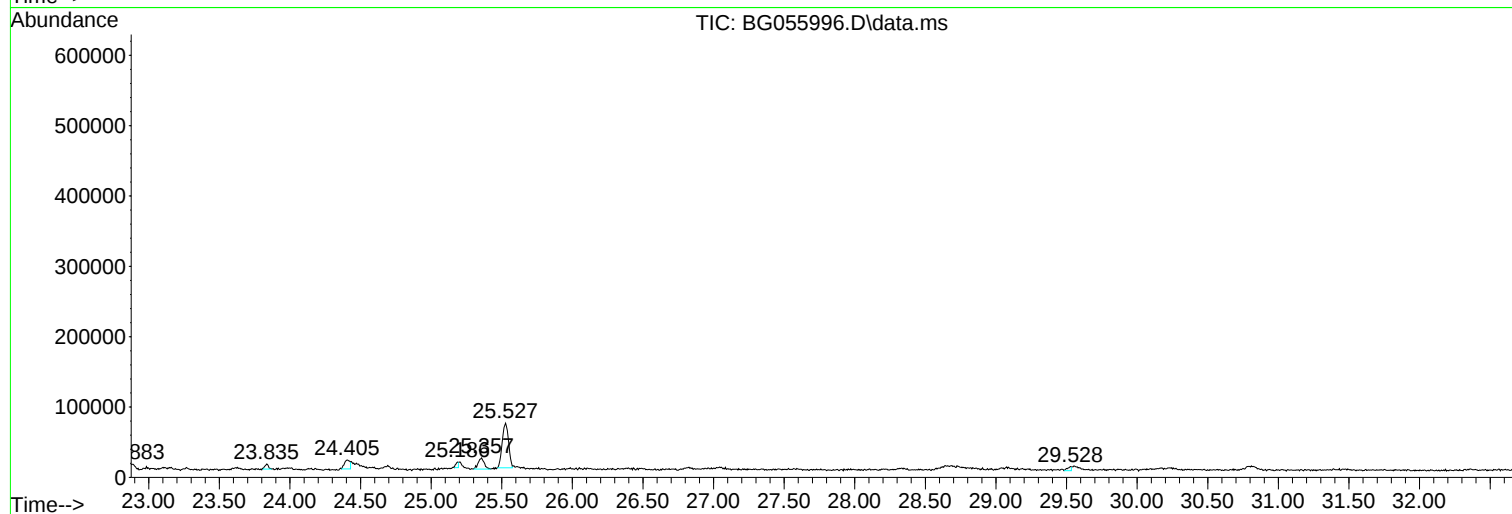
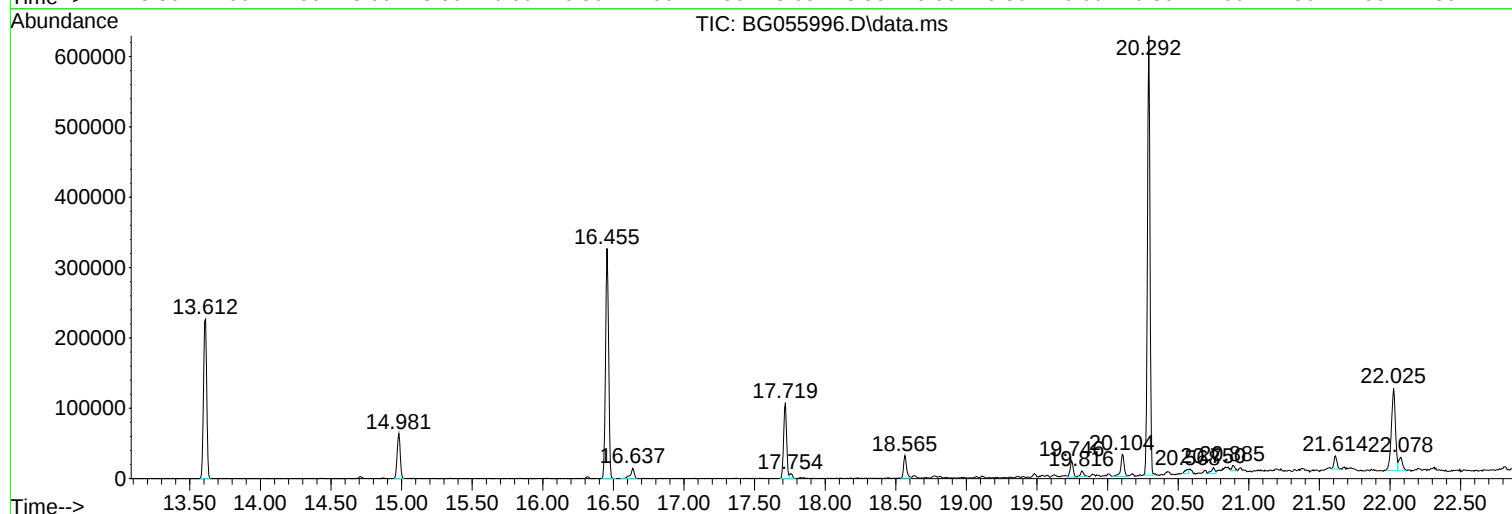
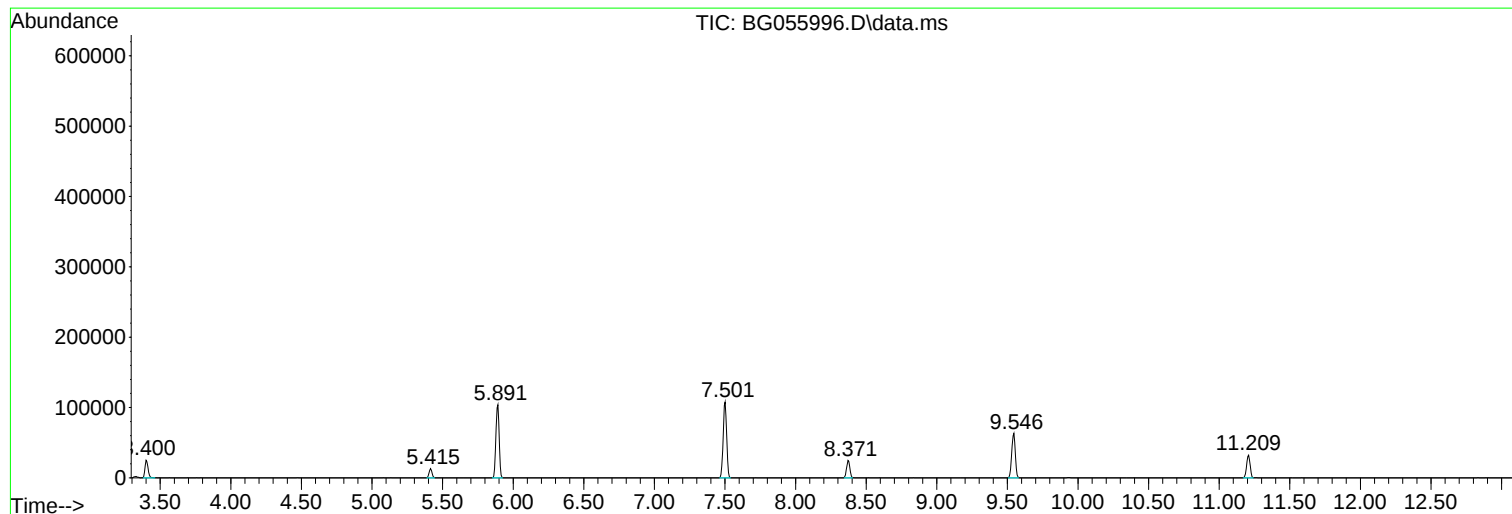
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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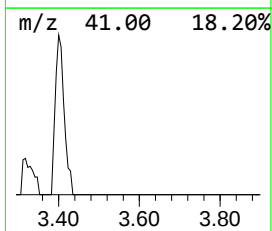
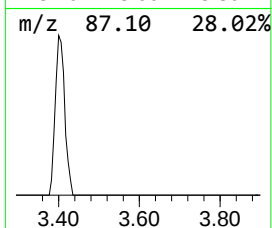
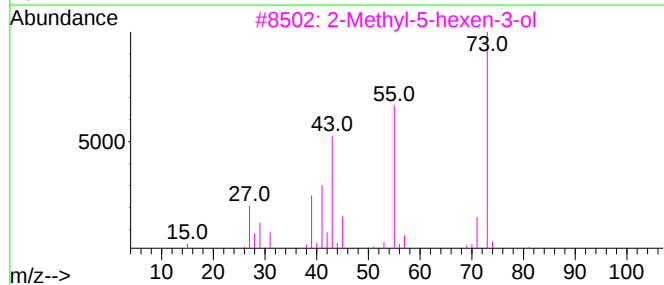
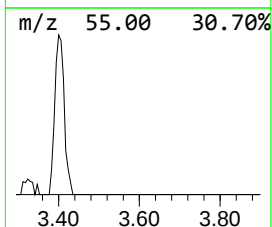
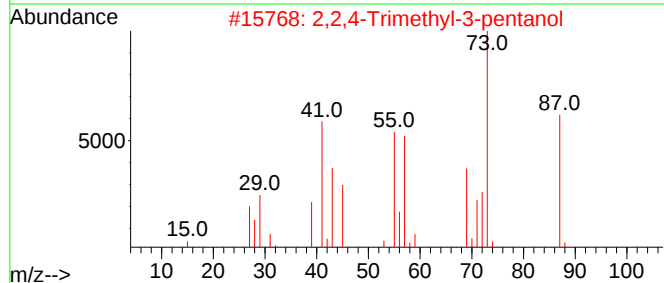
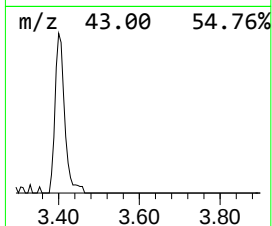
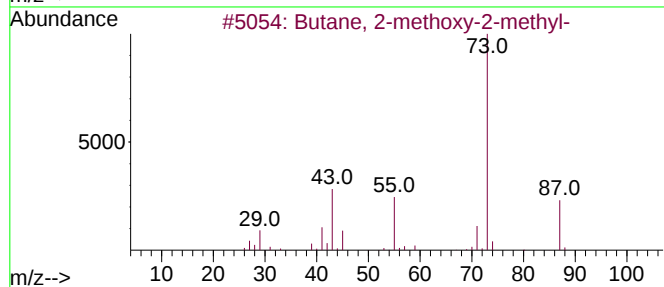
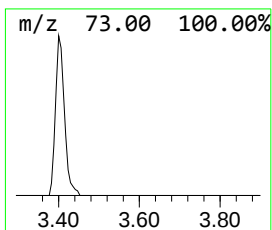
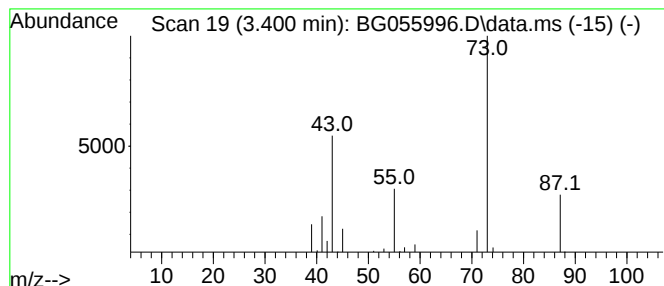
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.400	19.00 ng	38115	1,4-Dichlorobenzene-d4	8.371

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	38
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	25
4			Acetic acid, (acetyloxy)-	118	C4H6O4	013831-30-6	10
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	9



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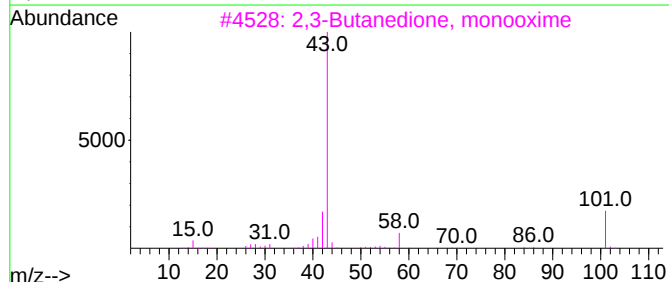
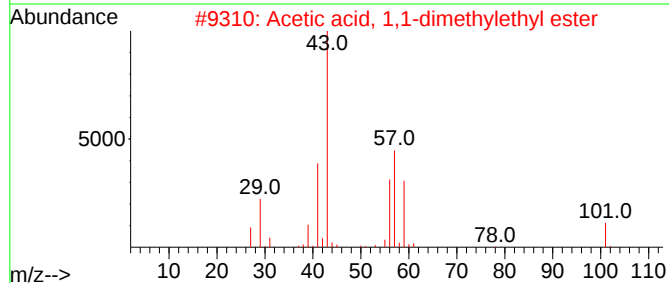
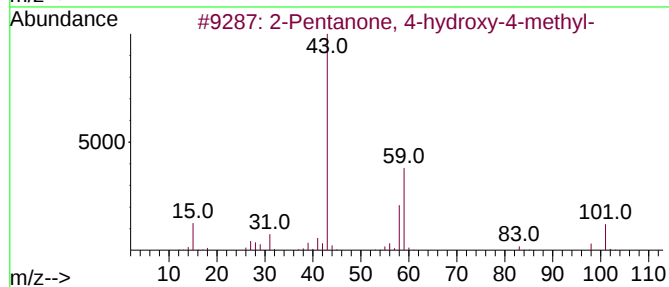
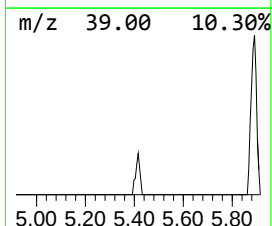
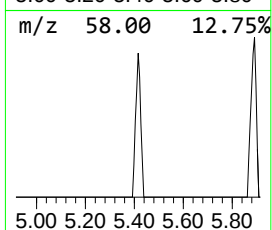
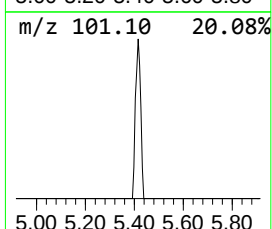
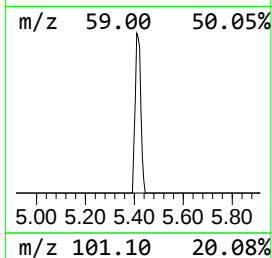
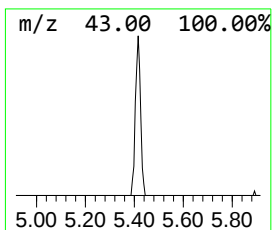
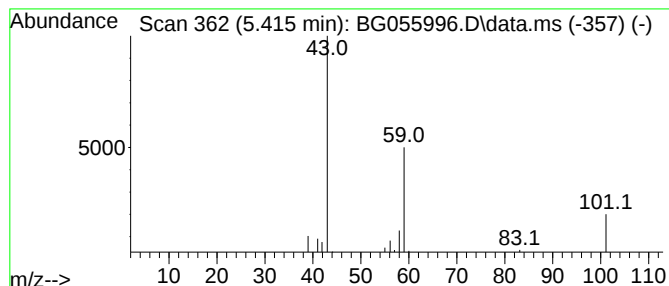
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.415	9.31 ng	18686	1,4-Dichlorobenzene-d4	8.371

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			N-(n-Propyl)acetamide	101	C5H11NO	005331-48-6	7



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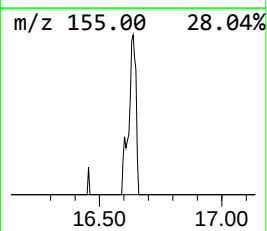
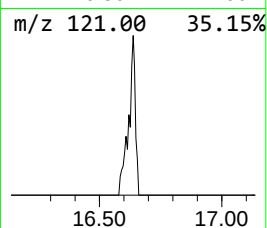
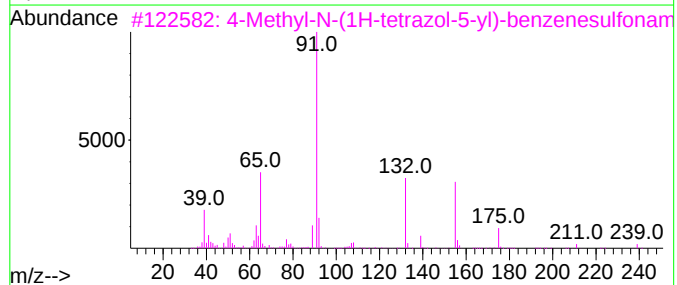
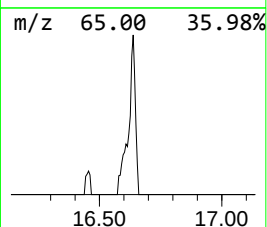
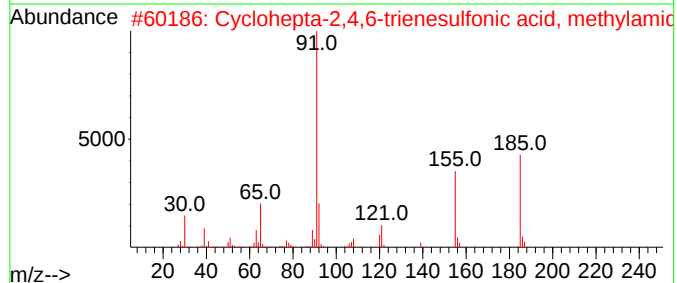
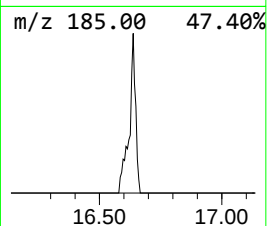
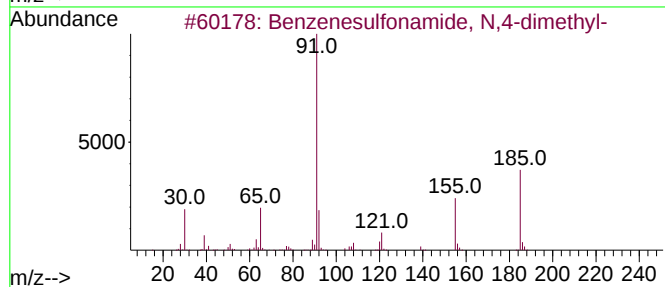
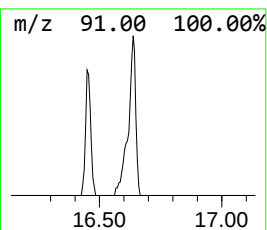
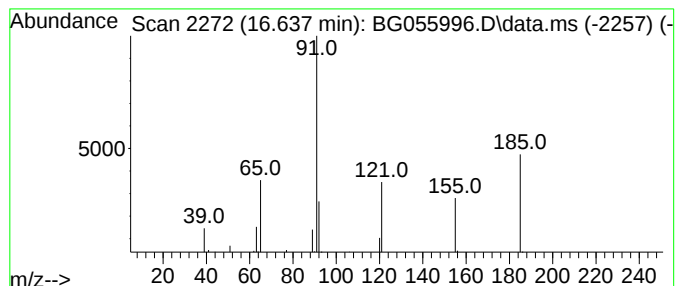
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzenesulfonamide, N,4-dim... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.637	3.47 ng	27788	Phenanthrene-d10	17.718

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzenesulfonamide, N,4-dimethyl-	185	C8H11NO2S	000640-61-9	86
2			Cyclohepta-2,4,6-trienesulfonic ...	185	C8H11NO2S	1000187-28-7	72
3			4-Methyl-N-(1H-tetrazol-5-yl)-be...	239	C8H9N5O2S	006455-80-7	43
4			Benzenesulfonic acid, 4-methyl-,...	186	C8H10O3S	000080-48-8	43
5			Benzenethanamine	121	C8H11N	000064-04-0	38



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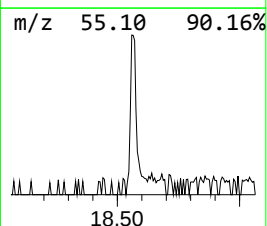
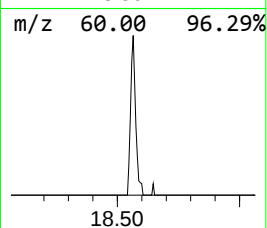
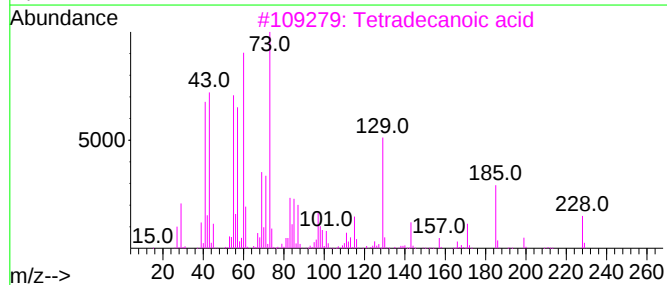
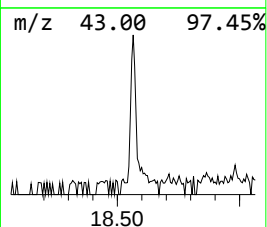
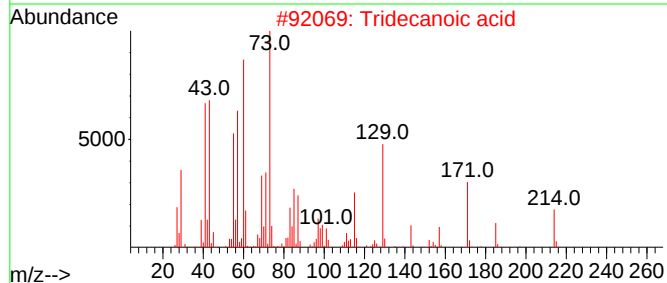
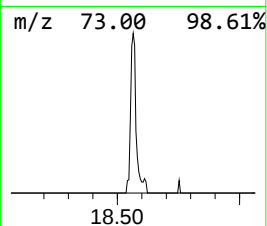
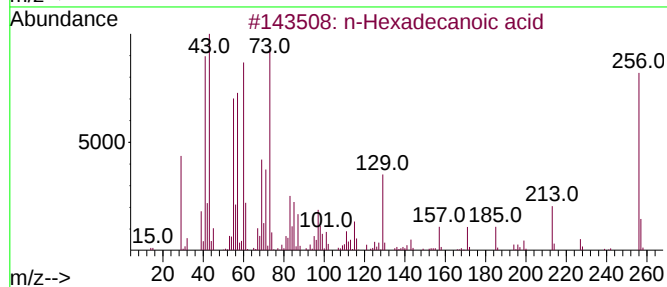
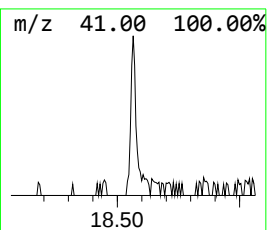
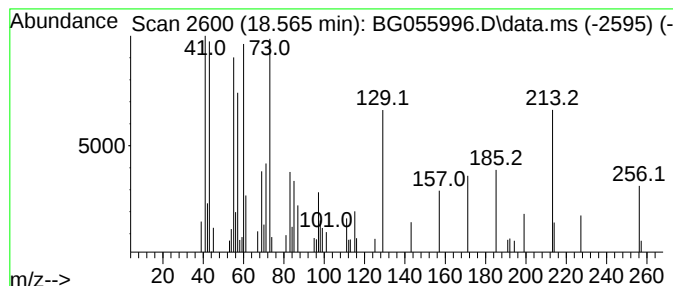
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.565	5.85 ng	46892	Phenanthrene-d10	17.718

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	55
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	52
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	45
5			Dodecanoic acid	200	C12H24O2	000143-07-7	43



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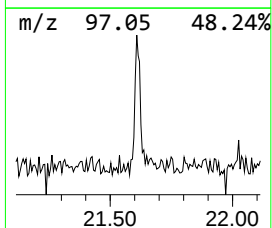
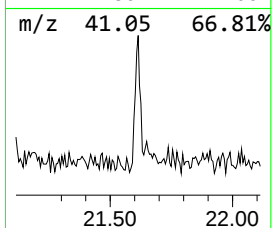
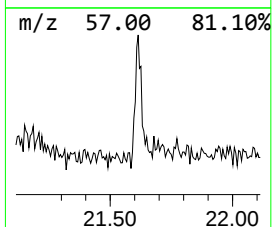
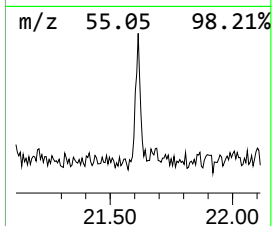
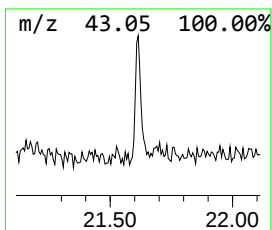
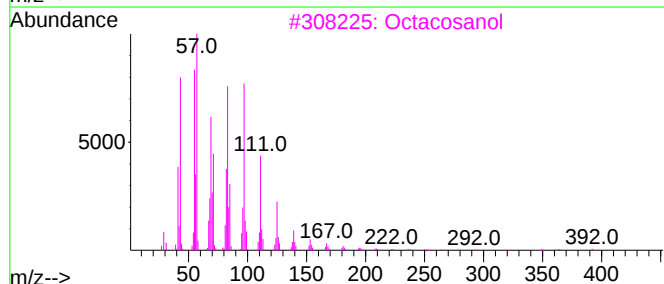
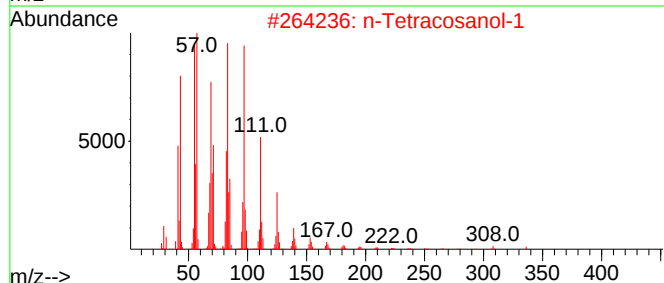
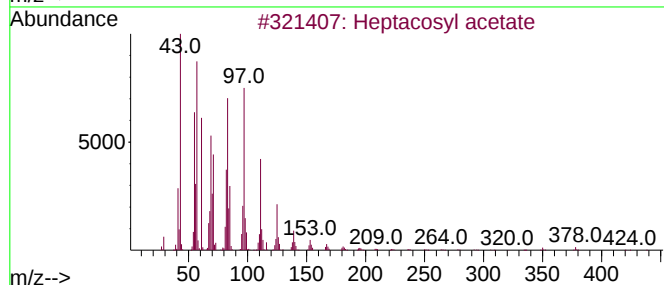
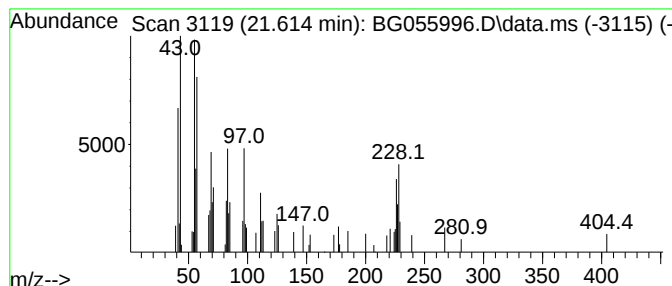
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Peak Number 5 Heptacosyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.614	2.35 ng	27375	Chrysene-d12	22.025

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	55
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	55
3			Octacosanol	410	C28H58O	000557-61-9	55
4			1-Hexacosene	364	C26H52	018835-33-1	55
5			Trifluoroacetic acid,n-tridecyl ...	296	C15H27F3O2	053800-02-5	53



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.400	19.0	ng	38115	1	8.371	40123	20.0
2-Pentanone, 4-...	5.415	9.3	ng	18686	1	8.371	40123	20.0
Benzenesulfonam...	16.637	3.5	ng	27788	4	17.718	160263	20.0
n-Hexadecanoic ...	18.565	5.8	ng	46892	4	17.718	160263	20.0
Heptacosyl acetate	21.614	2.4	ng	27375	5	22.025	232542	20.0