

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP012423\
 Data File : BP013568.D
 Acq On : 24 Jan 2023 13:25
 Operator : CG/JU
 Sample : 01214-18
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TJRC-011823-GW

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_P\Methods\8270E-BP012323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013568.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.223	3	6	29	rVB	4676395	5912071	44.99%	9.418%
2	5.217	339	345	355	rVB	606496	827947	6.30%	1.319%
3	5.687	418	425	436	rVB	1825216	2644452	20.12%	4.212%
4	7.293	690	698	709	rBV	987526	1599843	12.17%	2.548%
5	8.158	837	845	851	rBV	914767	1424859	10.84%	2.270%
6	9.328	1036	1044	1052	rBV	2573581	4364394	33.21%	6.952%
7	9.752	1109	1116	1122	rBV2	91728	168123	1.28%	0.268%
8	10.269	1197	1204	1218	rBV	81794	162746	1.24%	0.259%
9	10.987	1318	1326	1335	rBV	1098987	1910407	14.54%	3.043%
10	11.752	1449	1456	1470	rBV	73811	143118	1.09%	0.228%
11	13.422	1732	1740	1754	rBV	7022792	9963074	75.81%	15.871%
12	14.063	1841	1849	1866	rBV	304713	811969	6.18%	1.293%
13	14.793	1966	1973	1985	rVB	1536031	2289277	17.42%	3.647%
14	16.145	2197	2203	2211	rBV	780060	1042286	7.93%	1.660%
15	16.281	2218	2226	2236	rBV	4441817	6569919	49.99%	10.466%
16	17.545	2435	2441	2451	rBV	1841152	2613483	19.89%	4.163%
17	18.404	2582	2587	2597	rBV	209430	348245	2.65%	0.555%
18	19.628	2791	2795	2806	rBV2	127244	199815	1.52%	0.318%
19	20.075	2866	2871	2877	rBV	10477297	13141404	100.00%	20.934%
20	21.298	3075	3079	3087	rBV2	201852	288681	2.20%	0.460%
21	21.622	3129	3134	3147	rVB	2150077	2887996	21.98%	4.600%
22	22.957	3357	3361	3368	rVB	186245	294233	2.24%	0.469%
23	24.210	3567	3574	3584	rVB2	1538100	3168472	24.11%	5.047%

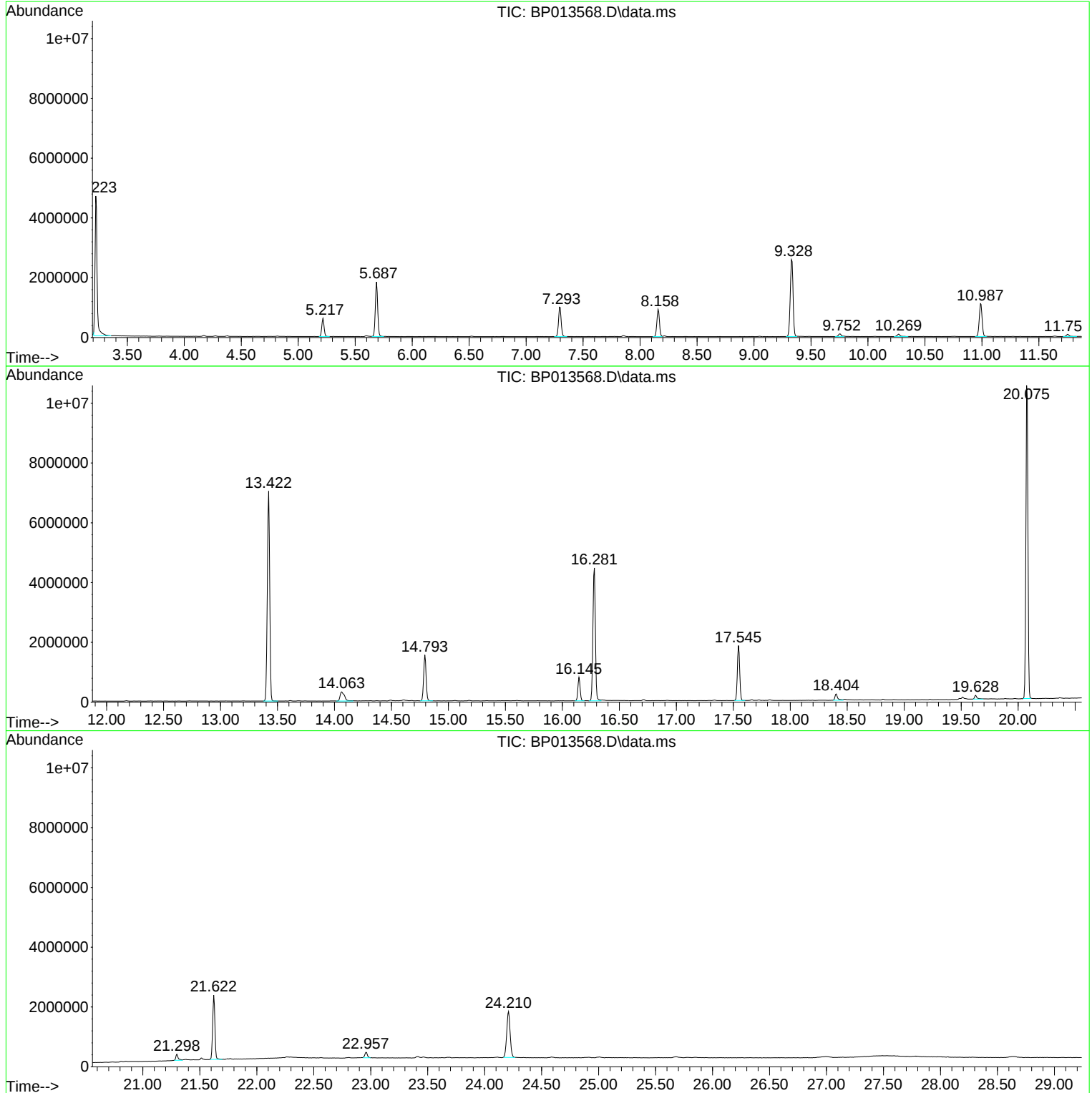
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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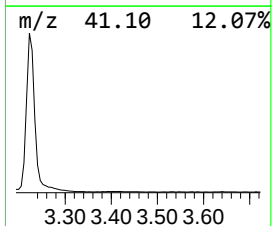
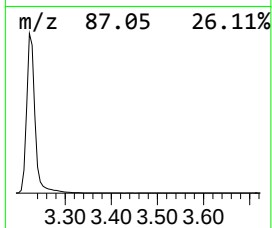
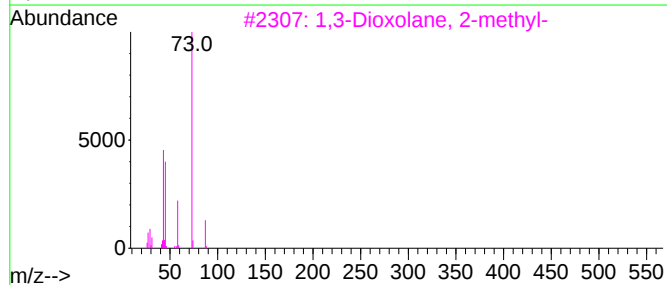
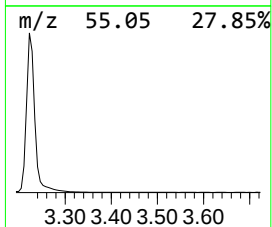
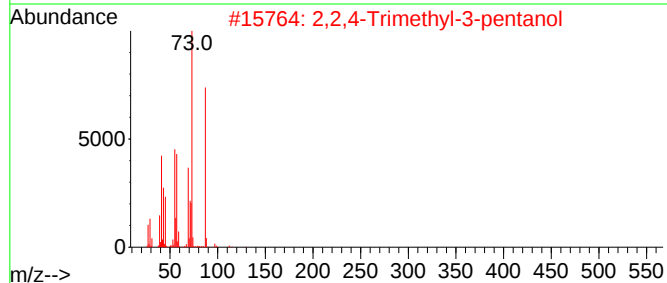
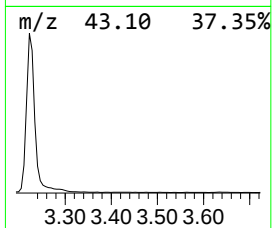
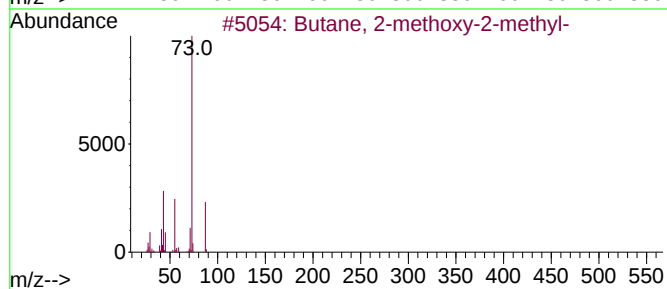
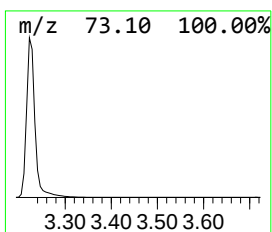
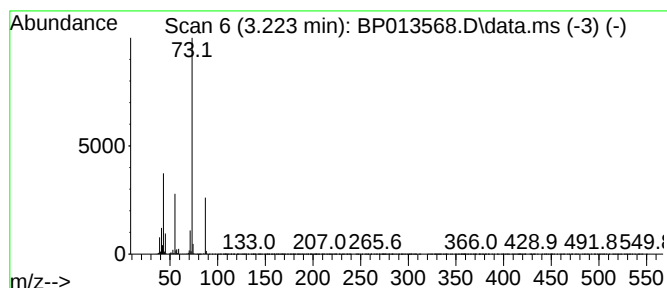
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP012323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.223	82.98 ng	5912070	1,4-Dichlorobenzene-d4	8.158

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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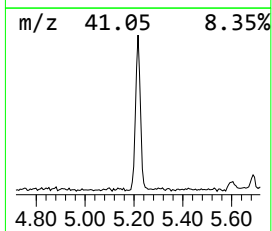
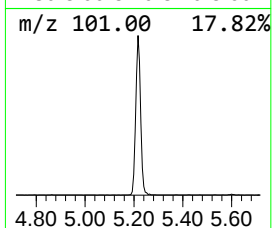
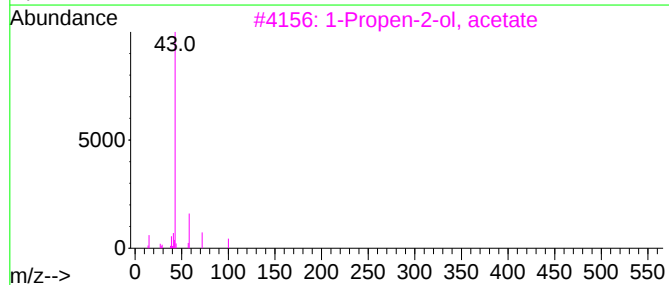
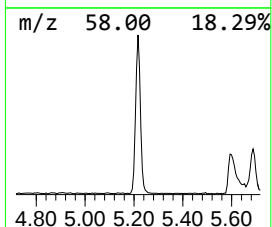
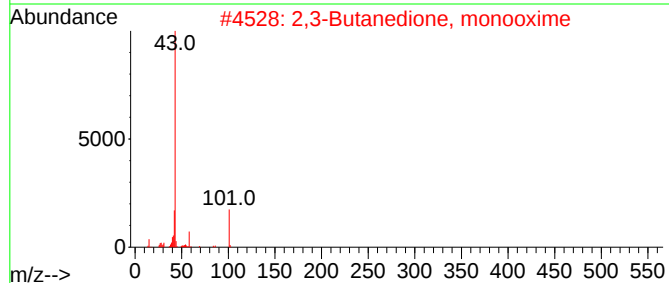
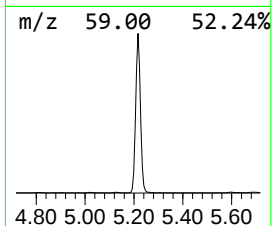
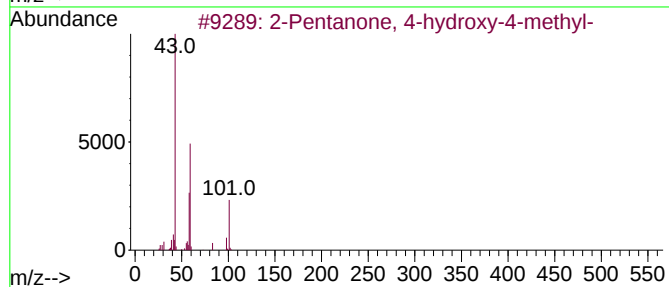
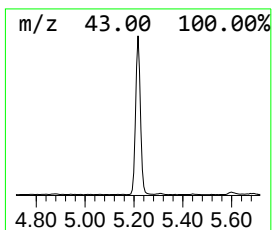
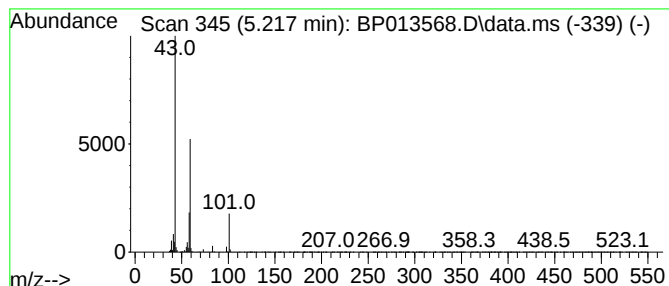
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.217	11.62 ng	827947	1,4-Dichlorobenzene-d4	8.158

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
4			Acetamide, N-(aminocarbonyl)-	102	C3H6N2O2	000591-07-1	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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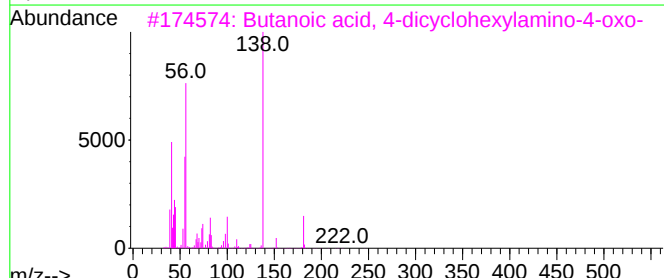
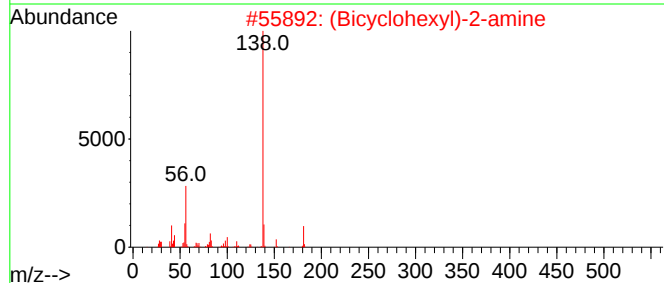
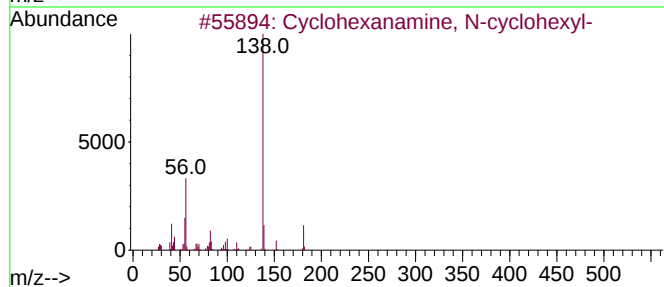
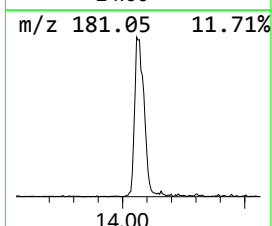
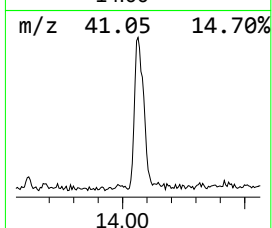
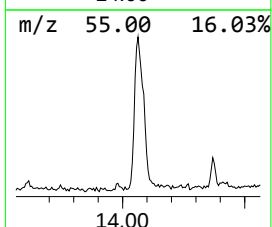
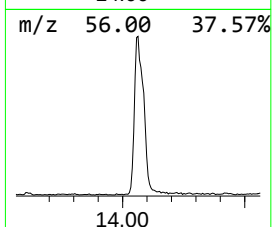
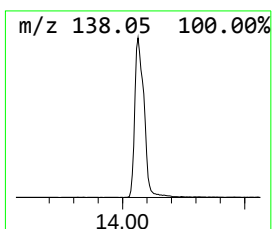
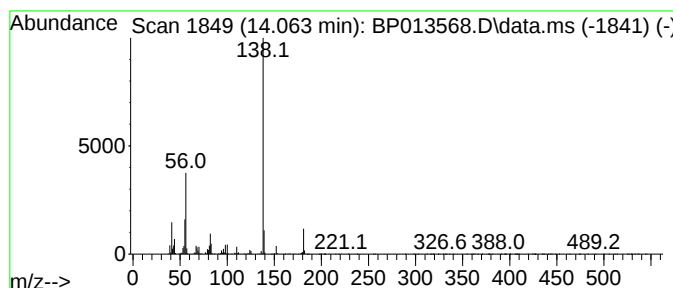
Instrument :
BNA_P
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TJRC-011823-GW

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

Peak Number 3 Cyclohexanamine, N-cyclohexyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.063	7.09 ng	811969	Acenaphthene-d10	14.793	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexanamine, N-cyclohexyl-	181	C12H23N	000101-83-7	96
2	(Bicyclohexyl)-2-amine	181	C12H23N	006283-14-3	96
3	Butanoic acid, 4-dicyclohexylami...	281	C16H27NO3	328013-95-2	64
4	4(1H)-Pyrimidinone, 2-ethyl-6-me...	138	C7H10N2O	016858-50-7	53
5	N-Butyl-1-cyclopropyl-2-methyl-5...	238	C13H22N2O2	1010458-31-0	53



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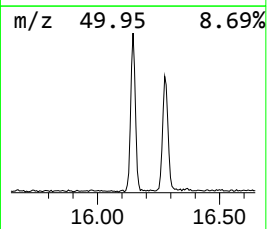
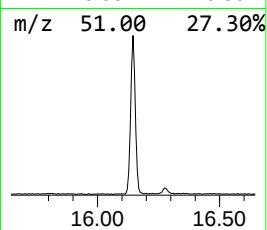
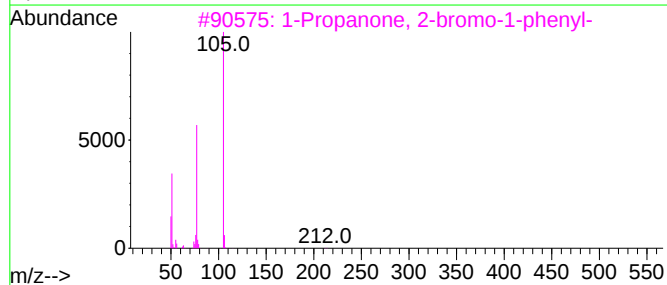
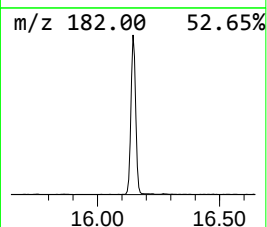
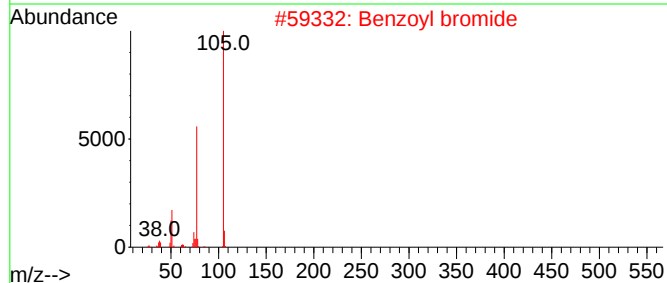
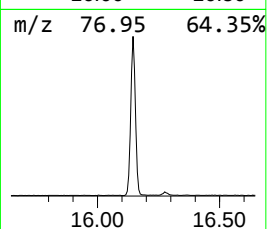
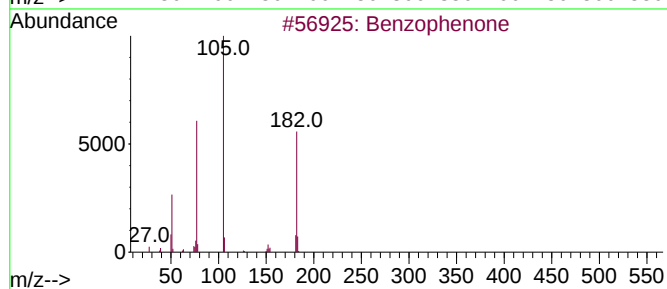
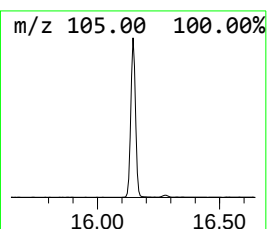
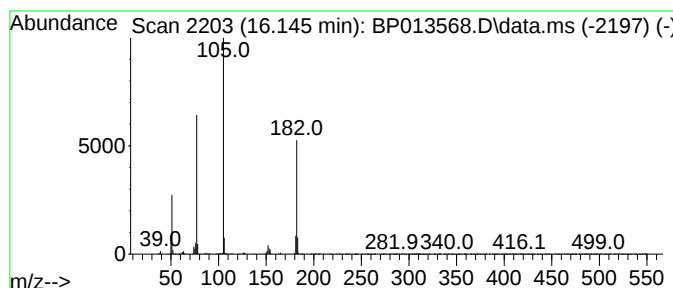
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.145	9.11 ng	1042290	Acenaphthene-d10	14.793

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzoyl bromide	184	C7H5BrO	000618-32-6	47
3			1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4			Benzoic acid, pentafluorophenyl ...	288	C13H5F5O2	1000360-67-9	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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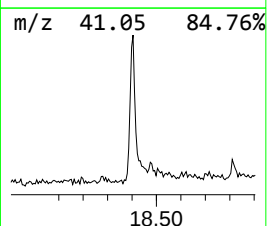
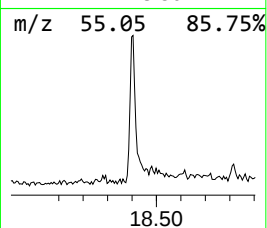
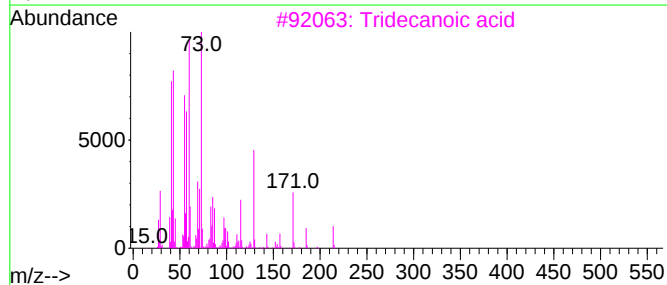
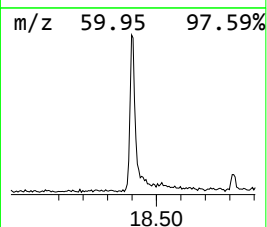
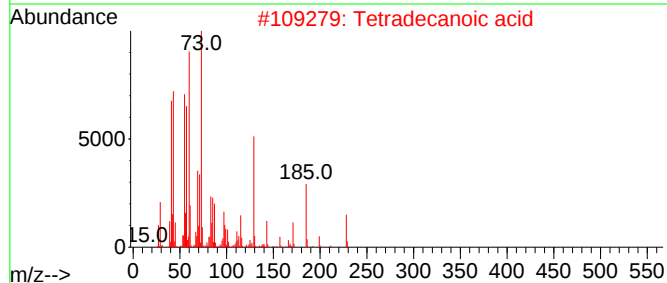
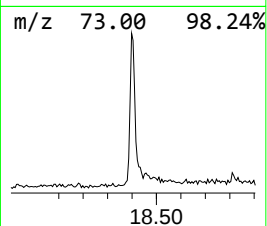
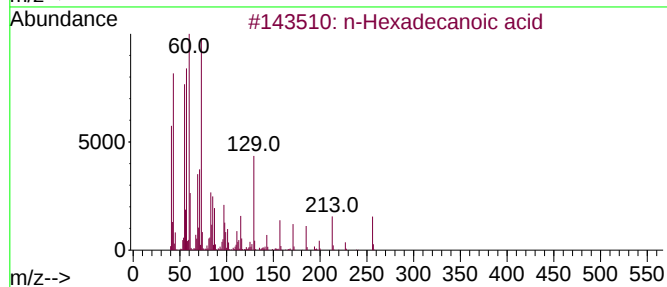
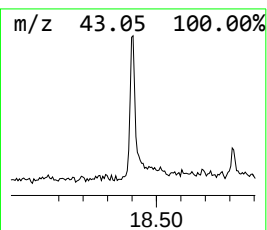
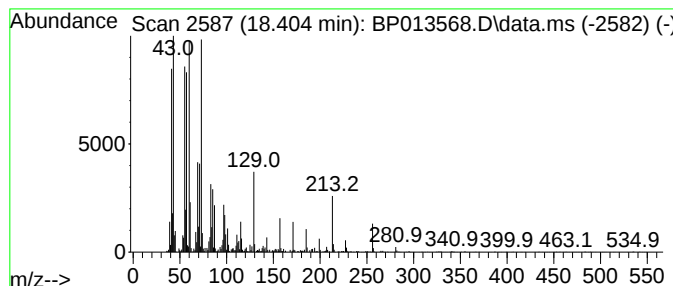
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.404	2.66 ng	348245	Phenanthrene-d10	17.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Octadecanoic acid	284	C18H36O2	000057-11-4	87



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.223	83.0	ng	5912070	1	8.158	1424860	20.0
2-Pentanone, 4-...	5.217	11.6	ng	827947	1	8.158	1424860	20.0
Cyclohexanamine...	14.063	7.1	ng	811969	3	14.793	2289280	20.0
Benzophenone	16.145	9.1	ng	1042290	3	14.793	2289280	20.0
n-Hexadecanoic ...	18.404	2.7	ng	348245	4	17.545	2613480	20.0