

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030725\
 Data File : BG064068.D
 Acq On : 7 Mar 2025 21:03
 Operator : RC/JU
 Sample : Q1514-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 ENV-103-GW01

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-BG030525.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG064068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.810	119	123	132	rVB	27951	44354	1.53%	0.398%
2	5.450	395	402	412	rBV	206628	314243	10.83%	2.819%
3	7.024	663	670	678	rBV	152635	259398	8.94%	2.327%
4	7.195	694	699	705	rBV3	18769	31892	1.10%	0.286%
5	7.865	806	813	820	rBV	150943	248759	8.57%	2.232%
6	9.016	1001	1009	1017	rVB	492995	867285	29.89%	7.781%
7	10.649	1280	1287	1295	rBV	207101	365108	12.58%	3.276%
8	13.111	1699	1706	1713	rBV	1292646	1962379	67.64%	17.605%
9	14.486	1932	1940	1947	rVB	351159	543947	18.75%	4.880%
10	15.843	2165	2171	2178	rBV	64314	96520	3.33%	0.866%
11	15.973	2187	2193	2201	rBV	646203	992183	34.20%	8.901%
12	17.160	2391	2395	2400	rVB	25890	32714	1.13%	0.293%
13	17.230	2400	2407	2413	rBV	445718	666852	22.99%	5.983%
14	18.129	2556	2560	2568	rBV2	63074	101541	3.50%	0.911%
15	19.410	2775	2778	2782	rBV3	20868	29450	1.02%	0.264%
16	19.545	2797	2801	2808	rBV2	43340	56900	1.96%	0.510%
17	19.645	2813	2818	2824	rBV7	19167	36524	1.26%	0.328%
18	19.850	2847	2853	2862	rBV	2230071	2901168	100.00%	26.028%
19	21.143	3069	3073	3079	rBV2	72938	109517	3.77%	0.983%
20	21.460	3120	3127	3138	rBV2	440309	724993	24.99%	6.504%
21	23.088	3400	3404	3410	rVB5	16651	30857	1.06%	0.277%
22	24.474	3630	3640	3651	rBV2	268037	729948	25.16%	6.549%

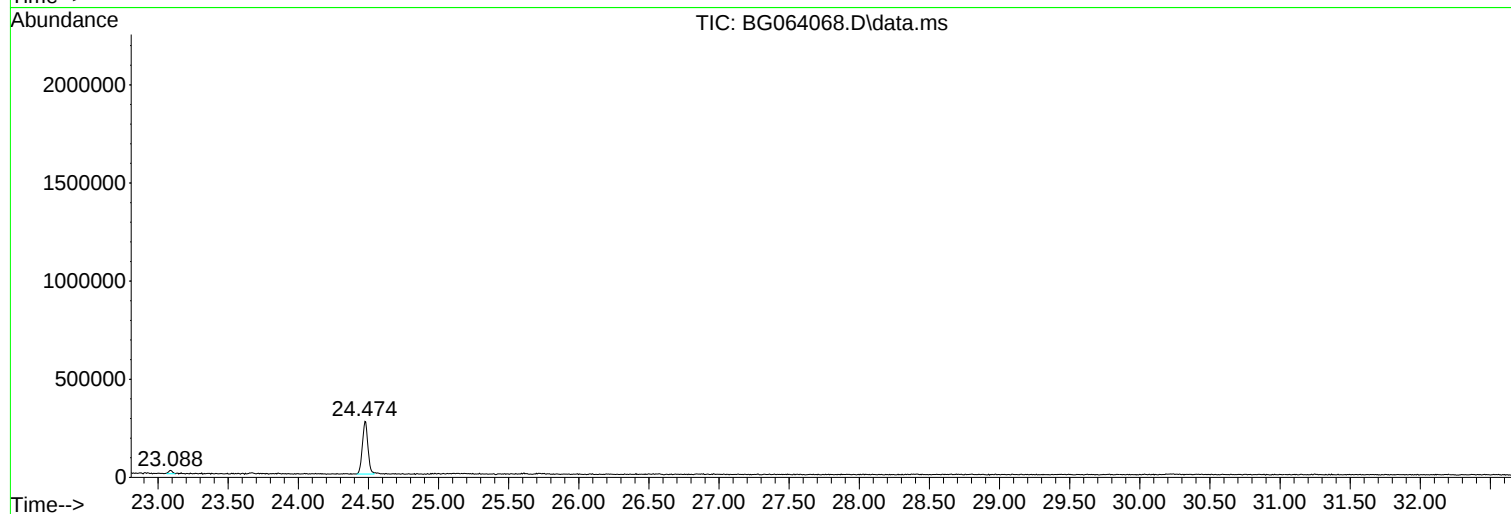
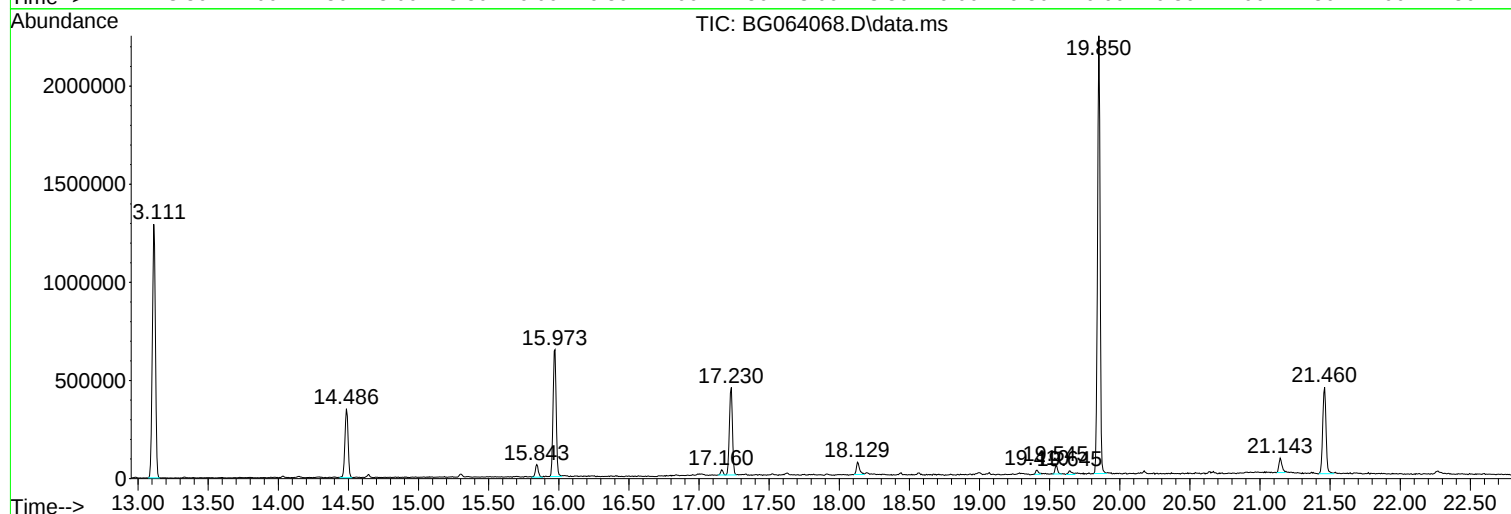
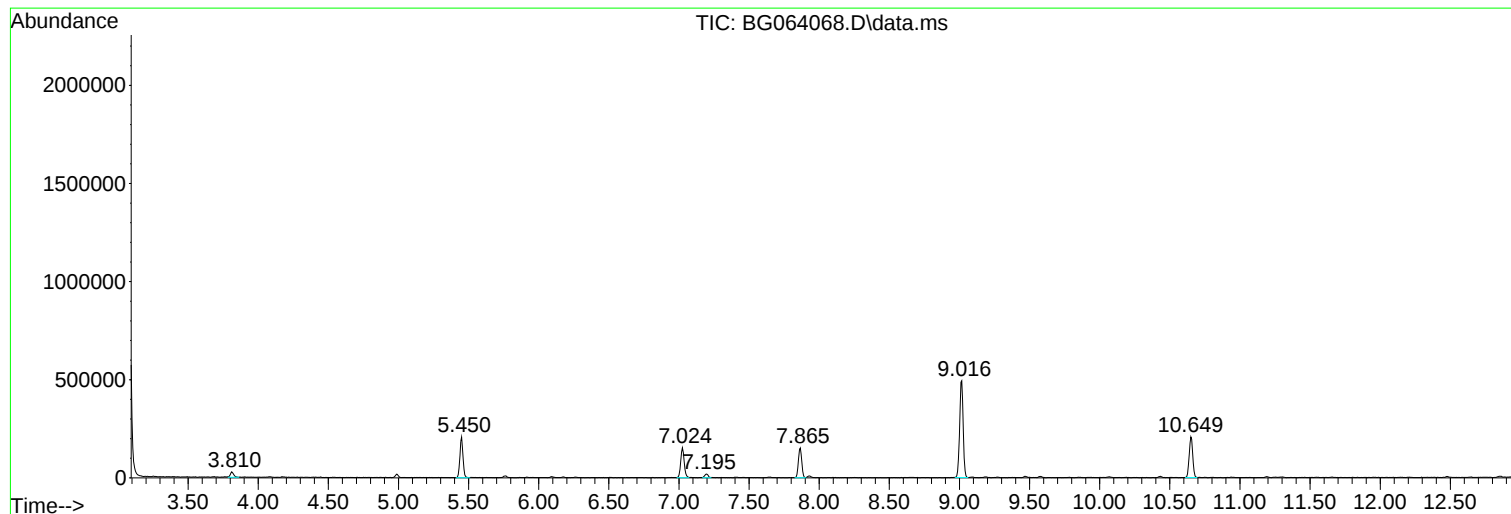
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Instrument :
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ClientSampleId :
ENV-103-GW01

Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG030525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG030725\
Data File : BG064068.D
Acq On : 7 Mar 2025 21:03
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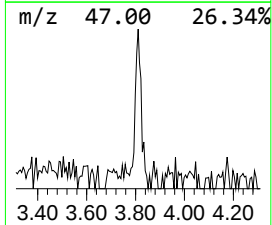
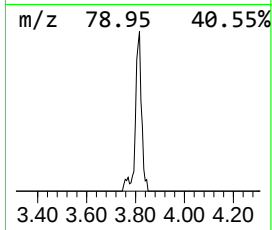
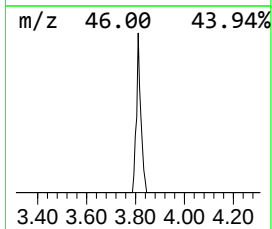
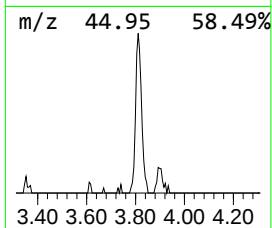
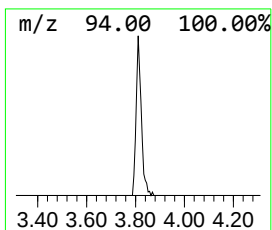
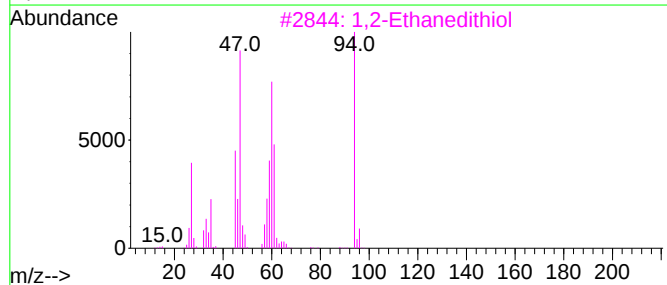
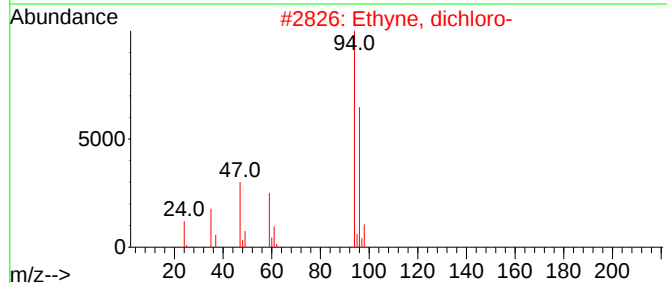
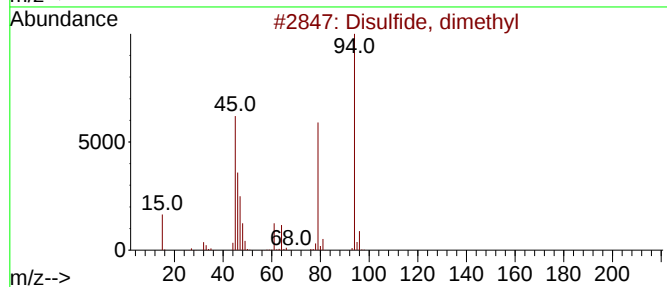
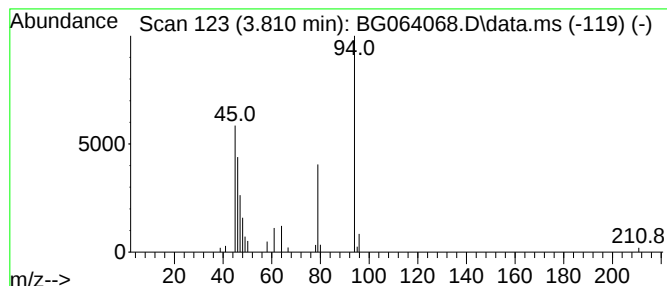
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.810	3.57 ng	44354	1,4-Dichlorobenzene-d4	7.864

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, dimethyl	94	C2H6S2	000624-92-0	87
2			Ethyne, dichloro-	94	C2Cl2	007572-29-4	35
3			1,2-Ethanedithiol	94	C2H6S2	000540-63-6	28
4			1,3,5,7-Tetrathiocane	184	C4H8S4	002373-00-4	12
5			Methyl 2-hydroxyethyl sulfoxide	108	C3H8O2S	021281-74-3	10



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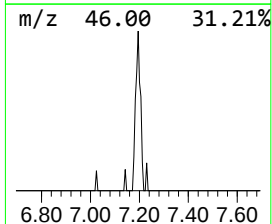
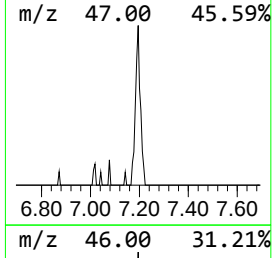
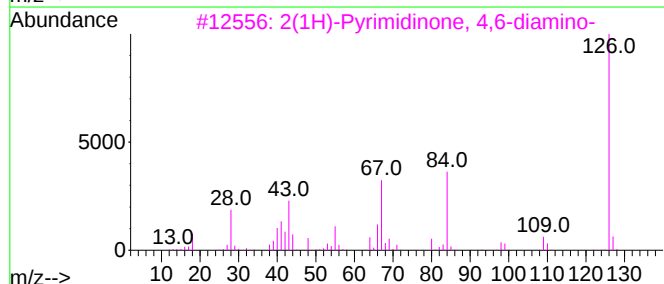
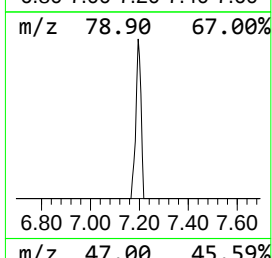
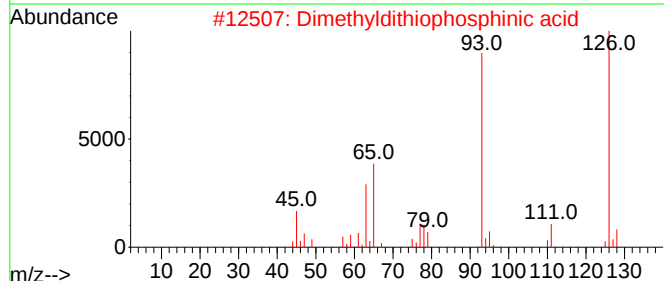
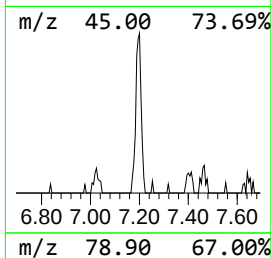
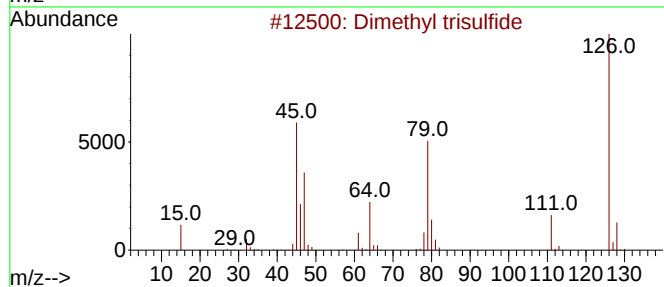
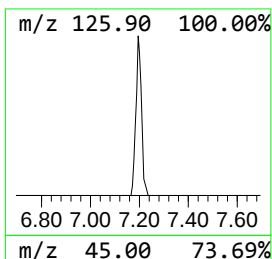
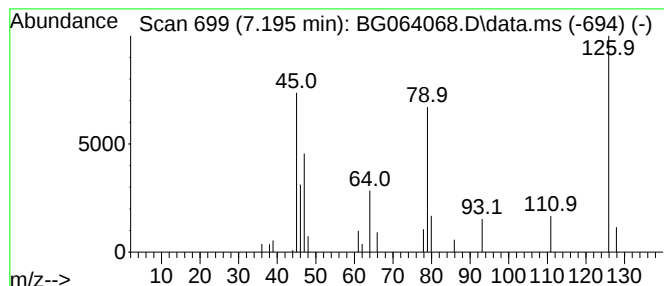
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Dimethyl trisulfide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.195	2.56 ng	31892	1,4-Dichlorobenzene-d4	7.864

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dimethyl trisulfide	126	C2H6S3	003658-80-8	94
2		Dimethyldithiophosphinic acid	126	C2H7PS2	016367-68-3	9
3		2(1H)-Pyrimidinone, 4,6-diamino-	126	C4H6N4O	031458-45-4	9
4		Butane, 4-chloro-1,1,1-trifluoro-	146	C4H6ClF3	000406-85-9	9
5		3-Nonyne, 9-methoxy-	154	C10H18O	054699-39-7	9



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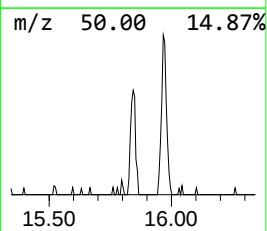
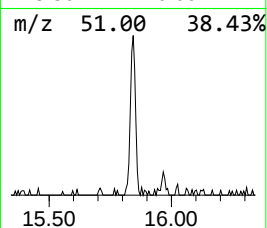
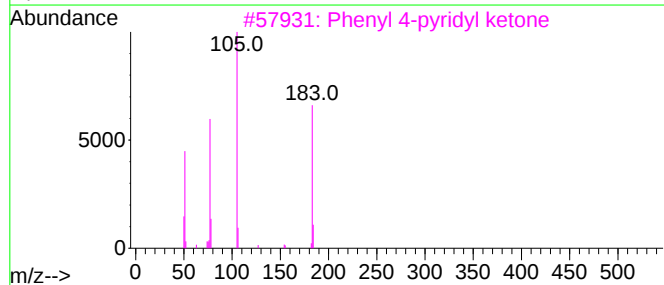
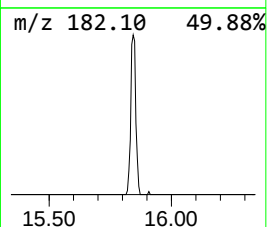
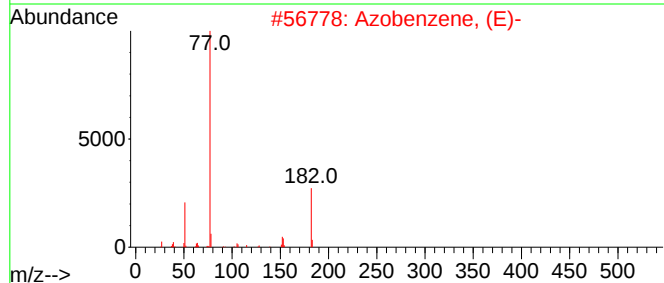
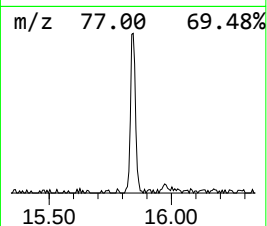
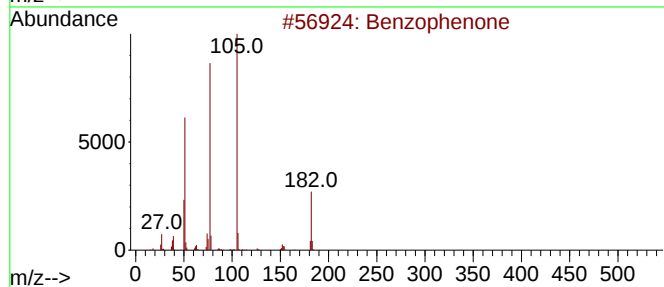
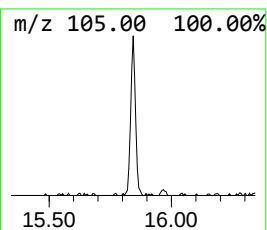
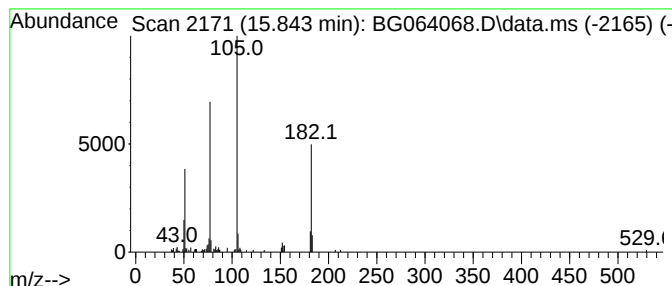
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.843	3.55 ng	96520	Acenaphthene-d10	14.486

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	50
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			Benzamide, N-(2-chloroacetyl)-	197	C9H8ClNO2	1000303-20-8	47
5			Benzoic acid, 2-propenyl ester	162	C10H10O2	000583-04-0	47



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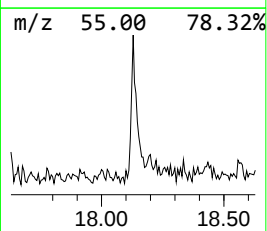
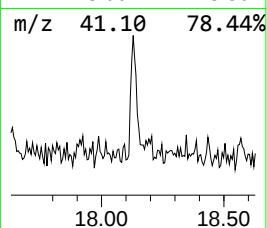
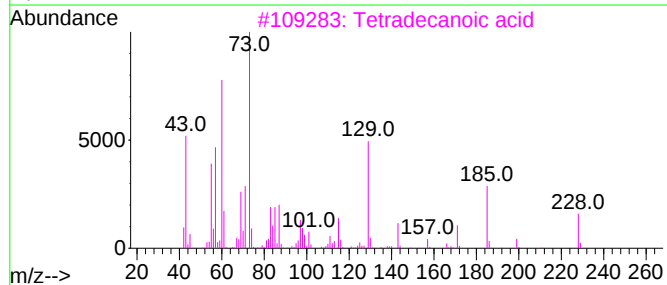
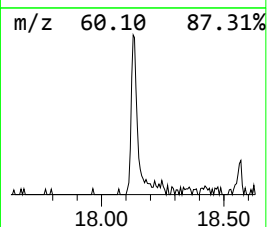
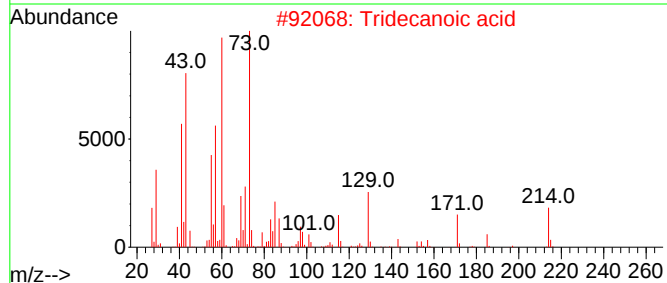
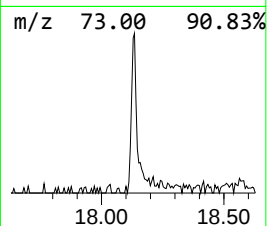
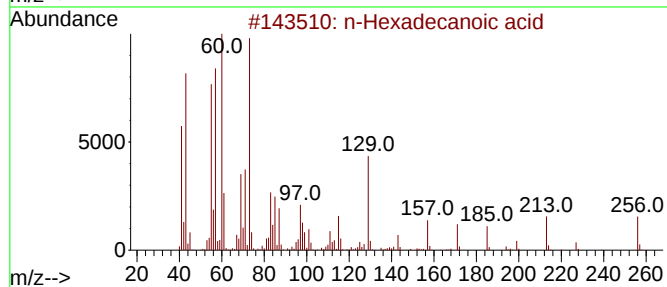
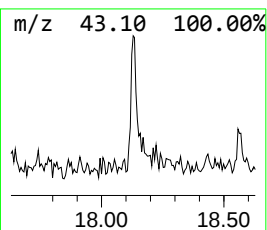
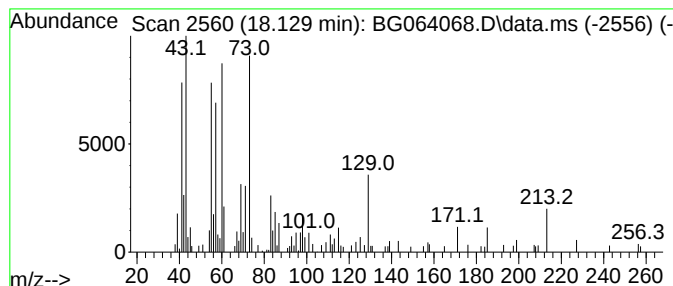
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.129	3.05 ng	101541	Phenanthrene-d10	17.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
2			Tridecanoic acid	214	C13H26O2	000638-53-9	72
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	59
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	59
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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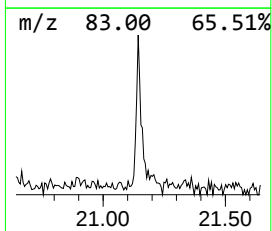
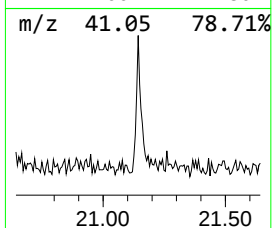
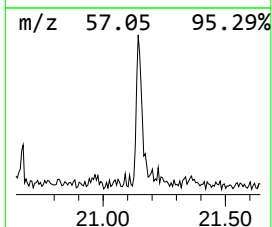
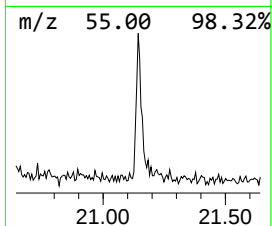
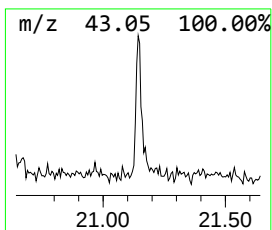
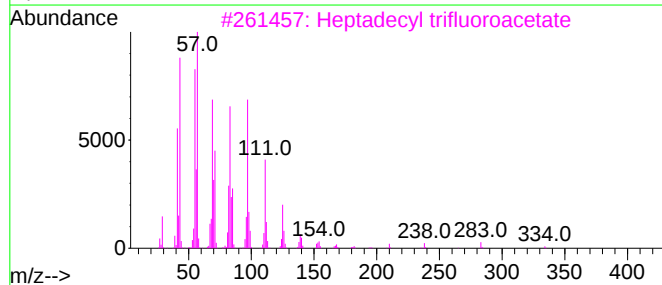
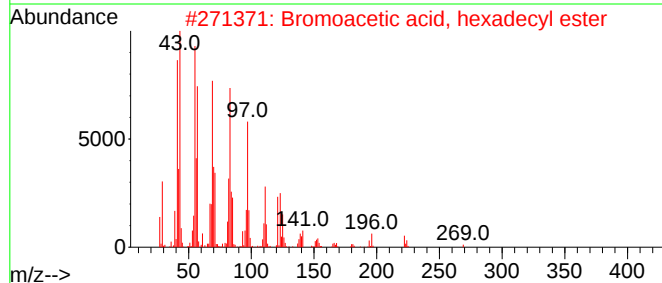
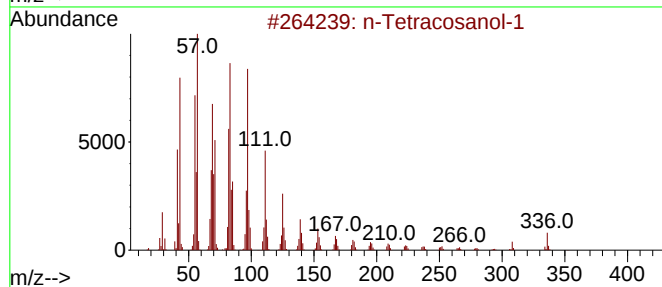
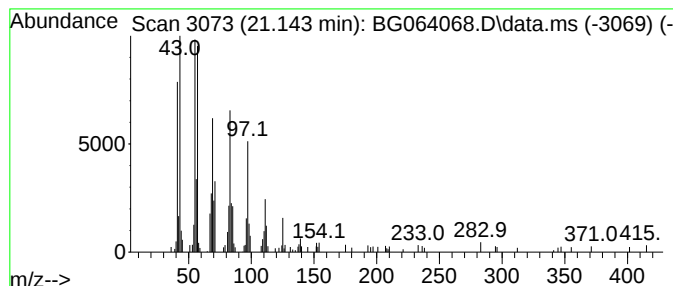
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.143	3.02 ng	109517	Chrysene-d12	21.460

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Tetracosanol-1	354	C24H50O	000506-51-4	91
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91
4			1-Tricosene	322	C23H46	018835-32-0	90
5			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	90



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Disulfide, dime...	3.810	3.6	ng	44354	1	7.864	248759	20.0
Dimethyl trisul...	7.195	2.6	ng	31892	1	7.864	248759	20.0
Benzophenone	15.843	3.5	ng	96520	3	14.486	543947	20.0
n-Hexadecanoic ...	18.129	3.0	ng	101541	4	17.230	666852	20.0
n-Tetracosanol-1	21.143	3.0	ng	109517	5	21.460	724993	20.0