

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM083024\
 Data File : BM047409.D
 Acq On : 30 Aug 2024 16:59
 Operator : RC/JU
 Sample : P3799-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TEST-PITS-3

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_M\Methods\8270-BM082624.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047409.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.557	277	284	291	rBV	168390	247132	3.52%	0.544%
2	5.005	353	360	383	rBV	2466797	3846082	54.84%	8.474%
3	6.569	619	626	652	rBV	2286970	3941893	56.21%	8.685%
4	7.346	750	758	768	rBV	750383	1228689	17.52%	2.707%
5	8.493	942	953	967	rBV	1539509	2679949	38.21%	5.905%
6	9.081	1046	1053	1066	rBV2	52677	140243	2.00%	0.309%
7	10.098	1217	1226	1241	rBV	911391	1612666	23.00%	3.553%
8	12.610	1646	1653	1671	rBV	3784729	5952311	84.88%	13.115%
9	14.004	1884	1890	1908	rVB	1375905	2195140	31.30%	4.836%
10	15.392	2120	2126	2139	rBV	1361944	1971925	28.12%	4.345%
11	15.521	2141	2148	2170	rVV	2889866	4567546	65.13%	10.064%
12	15.957	2215	2222	2232	rBV	169984	242679	3.46%	0.535%
13	16.774	2355	2361	2373	rBV	1610919	2481571	35.39%	5.468%
14	16.904	2379	2383	2393	rVB4	41522	70472	1.00%	0.155%
15	17.710	2515	2520	2542	rBV	700776	1239250	17.67%	2.730%
16	18.539	2657	2661	2666	rVB	48377	77291	1.10%	0.170%
17	18.857	2711	2715	2720	rBV	76776	134867	1.92%	0.297%
18	18.933	2725	2728	2734	rVV3	56977	106457	1.52%	0.235%
19	19.009	2737	2741	2753	rBV	234025	412850	5.89%	0.910%
20	19.227	2774	2778	2783	rVB	89854	117482	1.68%	0.259%
21	19.439	2809	2814	2827	rBV	5646004	7012827	100.00%	15.451%
22	20.745	3032	3036	3043	rBV	420925	603871	8.61%	1.330%
23	21.021	3078	3083	3088	rBV	1617323	2219766	31.65%	4.891%
24	23.721	3535	3542	3554	rVB	956929	2284105	32.57%	5.033%

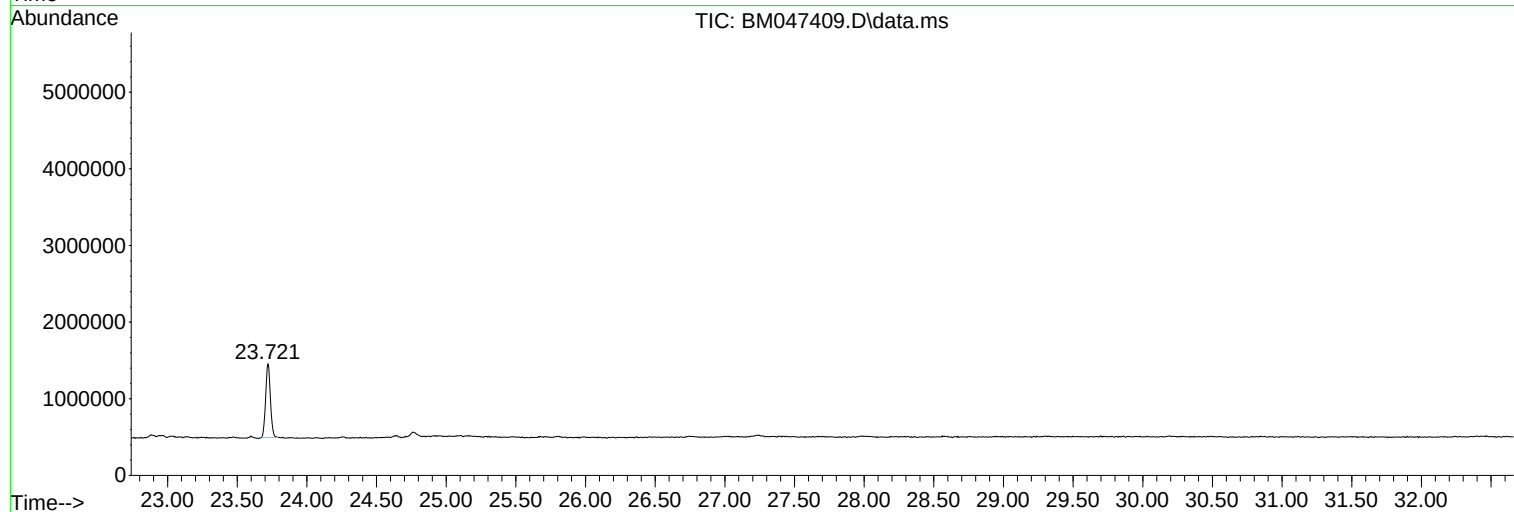
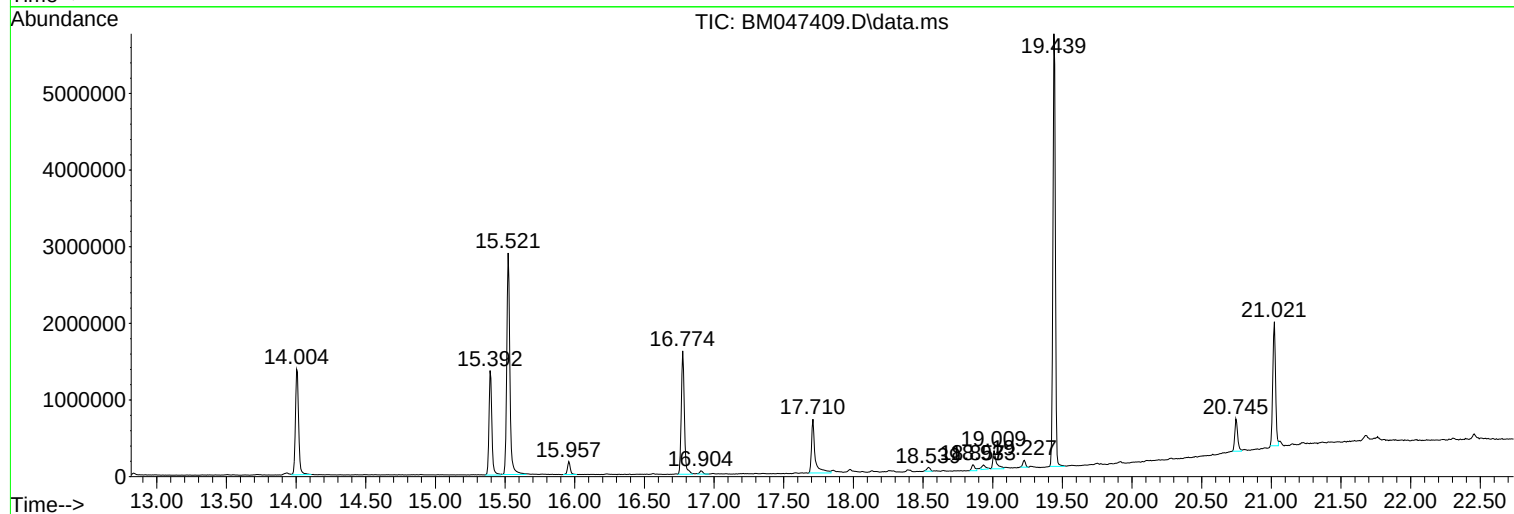
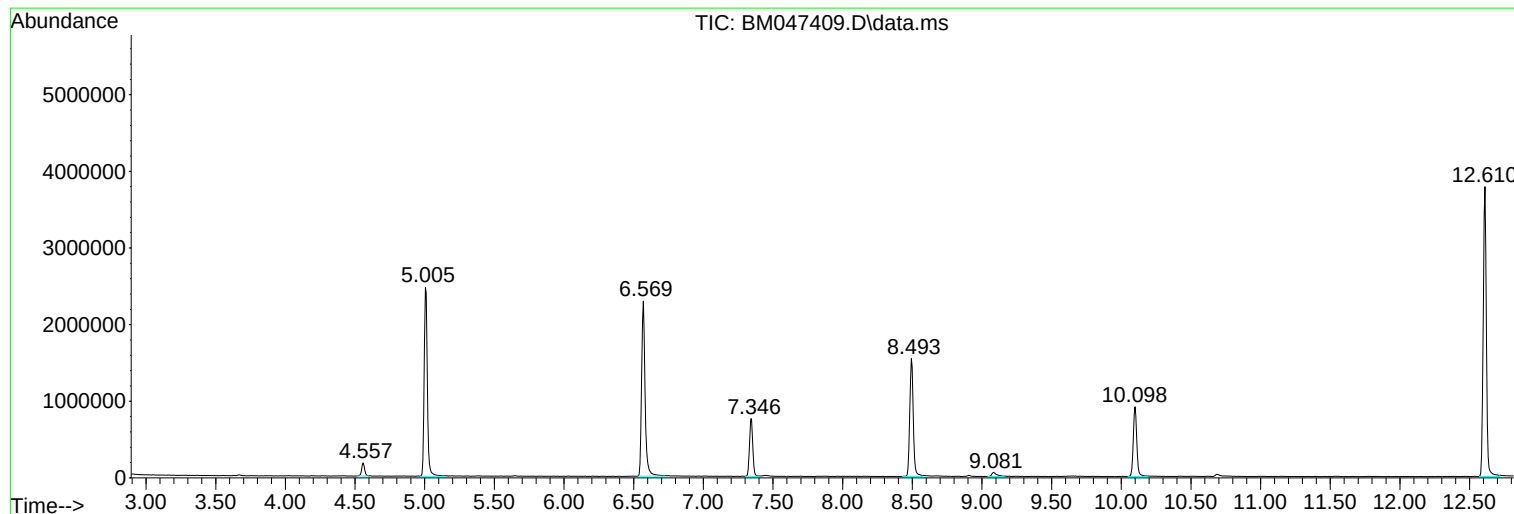
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM047409.D
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Instrument :
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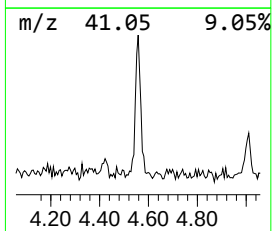
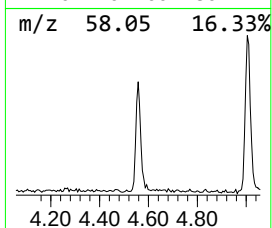
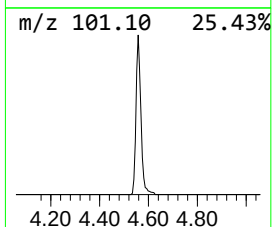
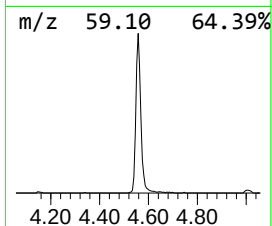
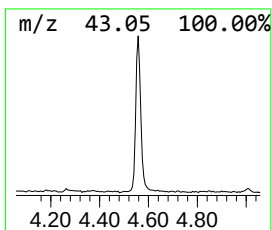
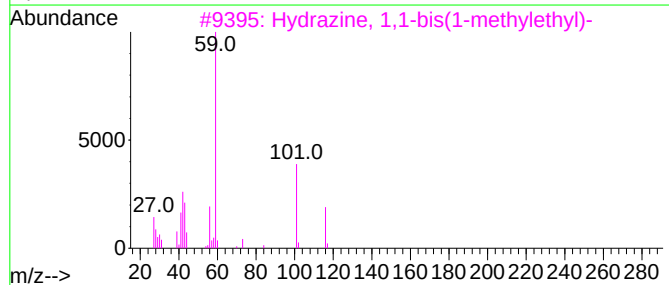
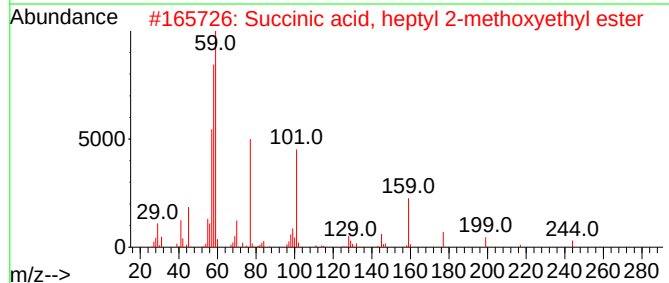
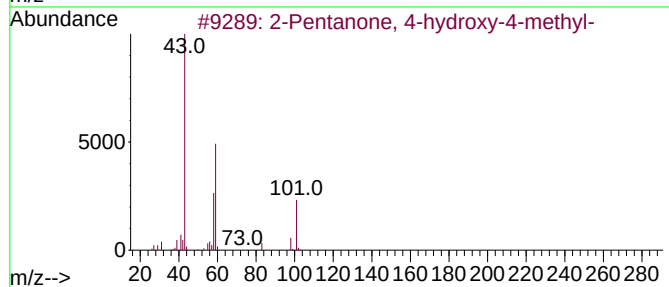
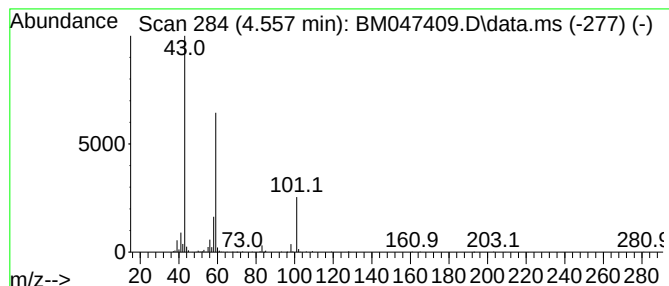
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	4.02 ng	247132	1,4-Dichlorobenzene-d4	7.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	33		
3	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		



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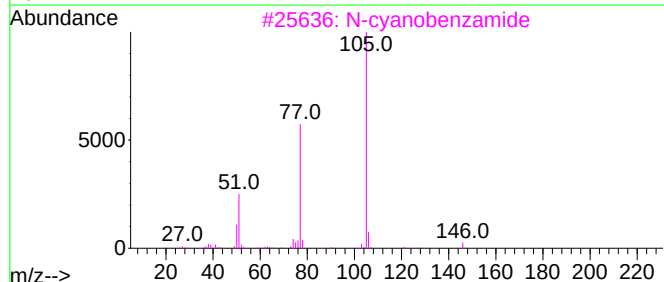
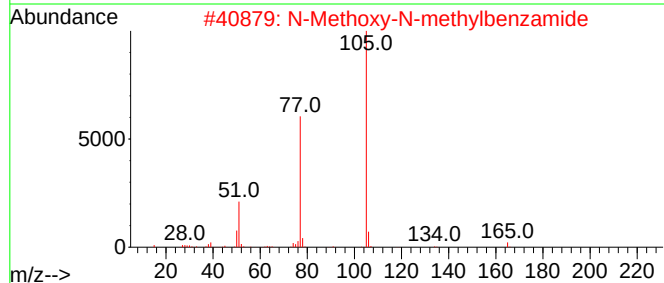
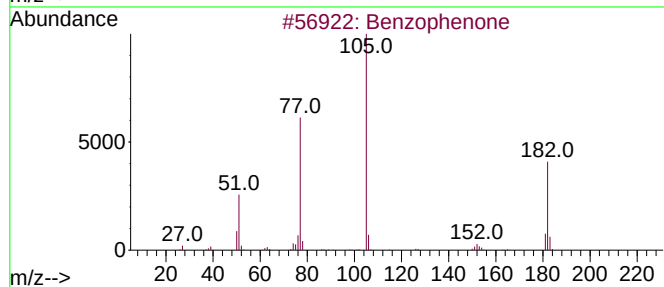
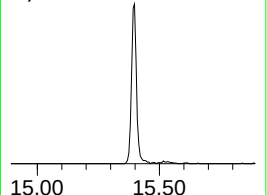
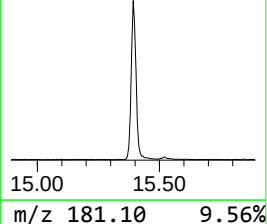
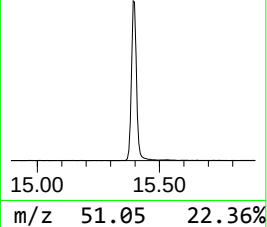
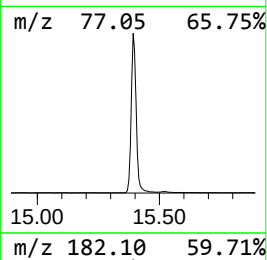
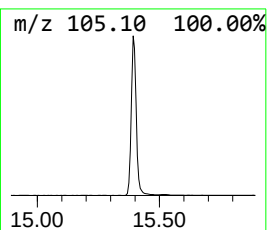
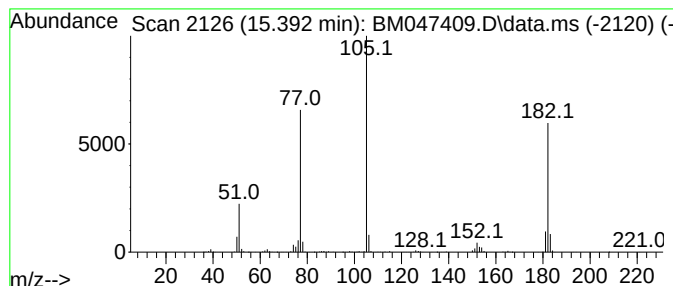
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.392	15.89 ng	1971930	Phenanthrene-d10	16.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	49
3			N-cyanobenzamide	146	C8H6N2O	015150-25-1	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47



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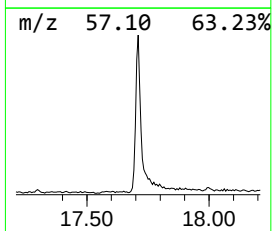
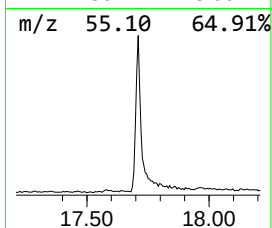
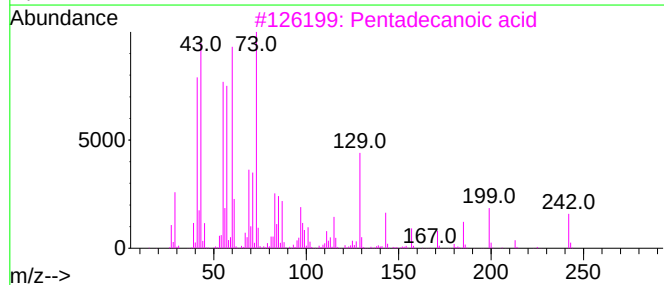
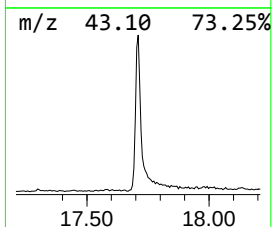
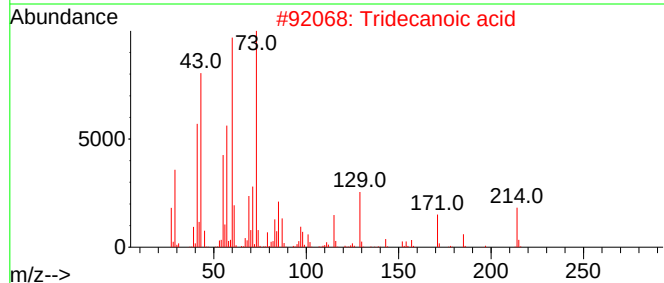
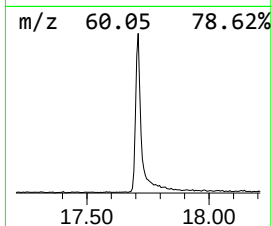
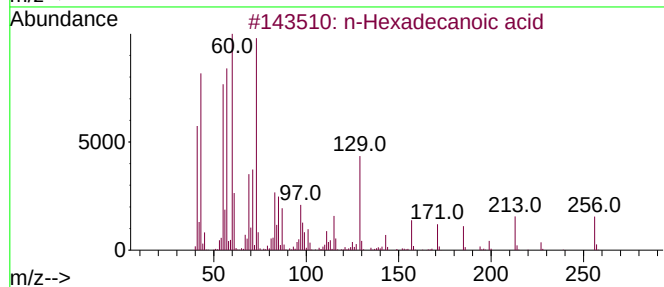
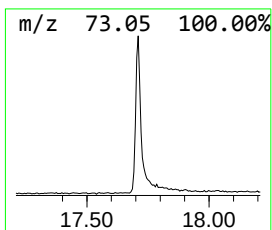
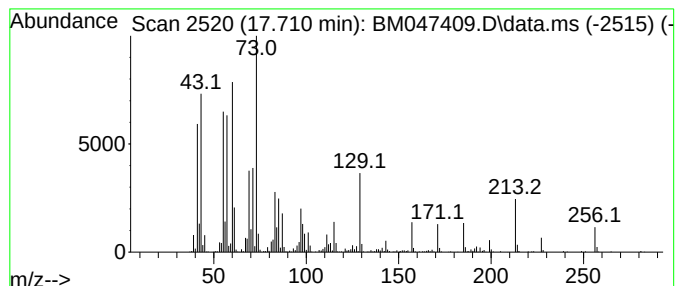
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BNA_M
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TEST-PITS-3

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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.710	9.99 ng	1239250	Phenanthrene-d10	16.774	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Nonanoic acid	158	C9H18O2	000112-05-0	38



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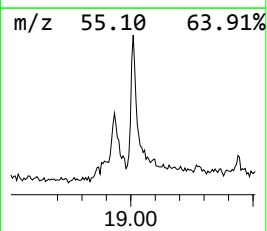
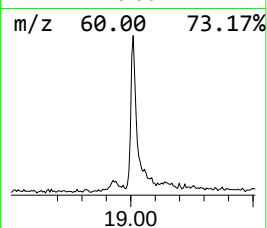
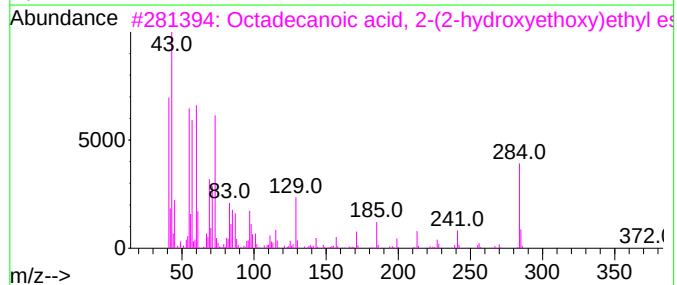
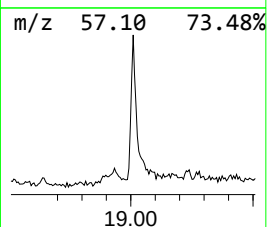
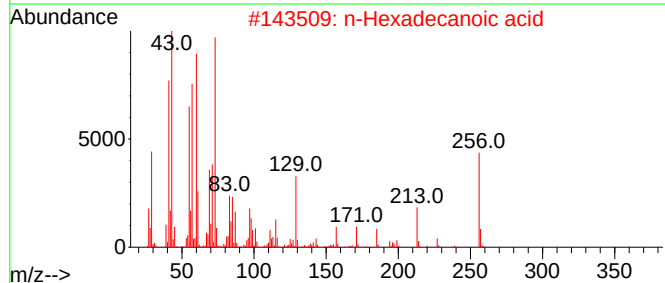
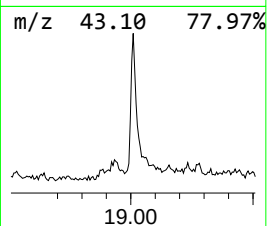
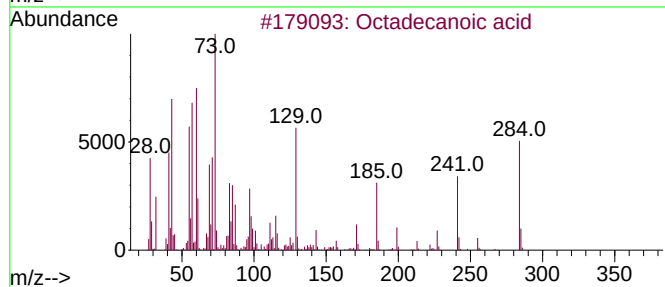
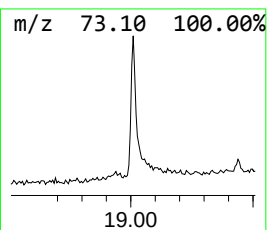
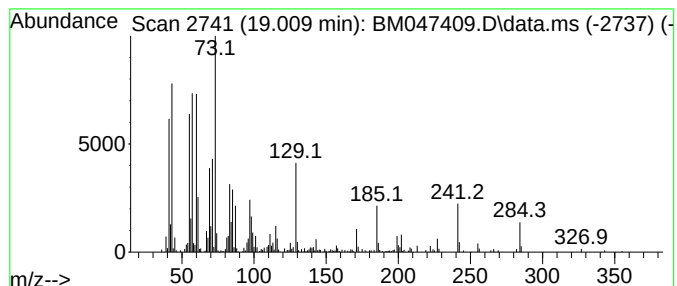
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	3.72 ng	412850	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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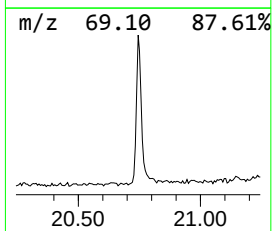
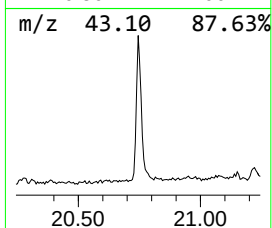
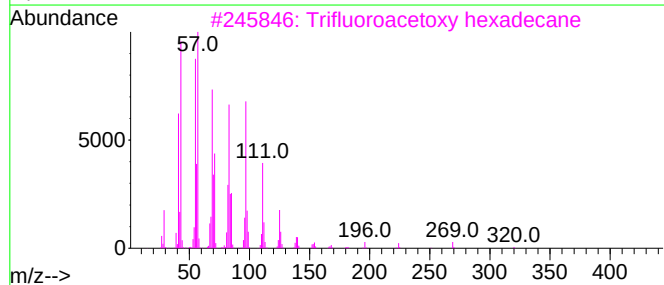
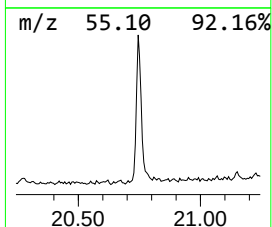
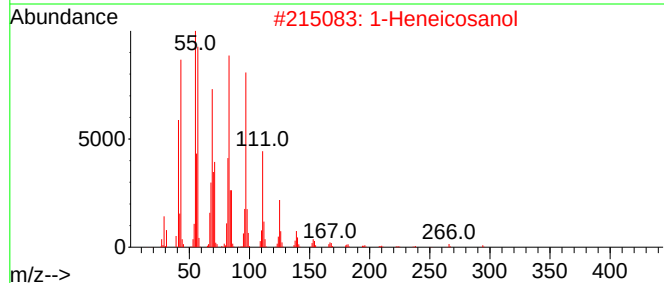
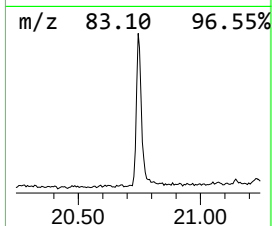
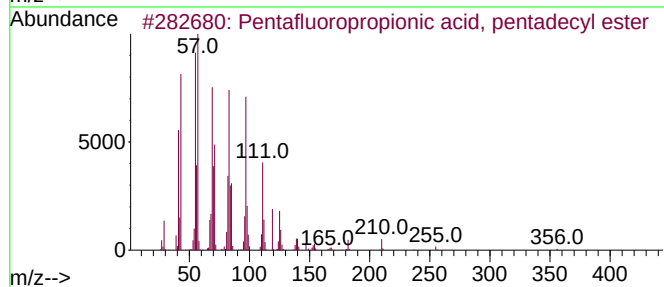
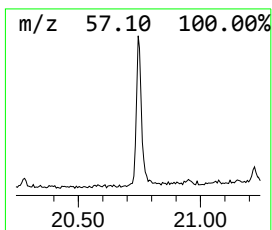
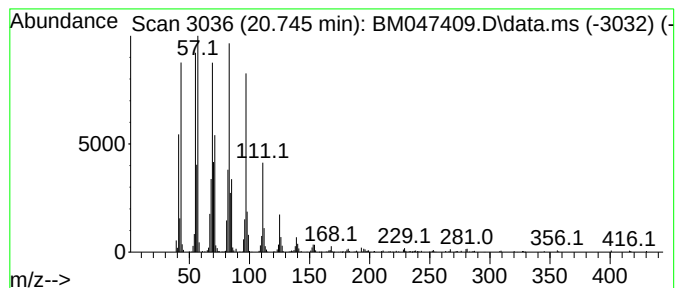
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Peak Number 5 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.745	5.44 ng	603871	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
2			1-Heneicosanol	312	C21H44O	015594-90-8	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
5			1-Tetracosene	336	C24H48	010192-32-2	91



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.557	4.0	ng	247132	1	7.346	1228690	20.0
Benzophenone	15.392	15.9	ng	1971930	4	16.774	2481570	20.0
n-Hexadecanoic ...	17.710	10.0	ng	1239250	4	16.774	2481570	20.0
Octadecanoic acid	19.009	3.7	ng	412850	5	21.021	2219770	20.0
Pentafluoroprop...	20.745	5.4	ng	603871	5	21.021	2219770	20.0