

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
 Data File : BM047300.D
 Acq On : 21 Aug 2024 16:26
 Operator : RC/JU
 Sample : P3596-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 918-J-WS-081324

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-BM081024.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047300.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.010	355	361	376	rBV	1266666	1885349	13.97%	3.368%
2	6.569	620	626	637	rBV	732596	1206879	8.94%	2.156%
3	7.351	752	759	769	rBV	655735	1042567	7.72%	1.863%
4	8.498	946	954	967	rBV	1698504	2837507	21.02%	5.069%
5	10.110	1221	1228	1239	rBV	790670	1352457	10.02%	2.416%
6	10.875	1352	1358	1369	rBV	79515	180181	1.33%	0.322%
7	12.622	1647	1655	1675	rBV	4217885	6546411	48.50%	11.695%
8	14.016	1885	1892	1909	rBV	1183622	1868991	13.85%	3.339%
9	14.251	1926	1932	1934	rBV	2937005	4345248	32.19%	7.763%
10	14.274	1934	1936	1953	rVB	3698940	4081143	30.23%	7.291%
11	15.521	2142	2148	2160	rBV	4429675	6608264	48.96%	11.806%
12	16.780	2356	2362	2371	rBV	1578418	2363679	17.51%	4.223%
13	17.715	2515	2521	2529	rBV	550704	854409	6.33%	1.526%
14	18.592	2665	2670	2676	rBV3	76581	141677	1.05%	0.253%
15	18.674	2680	2684	2688	rVB	192453	223966	1.66%	0.400%
16	19.015	2738	2742	2754	rBV2	248731	424525	3.15%	0.758%
17	19.451	2810	2816	2826	rBV	10882030	13498377	100.00%	24.115%
18	20.756	3034	3038	3050	rBV	371813	643520	4.77%	1.150%
19	21.021	3078	3083	3097	rBV	2181015	2982880	22.10%	5.329%
20	23.709	3533	3540	3554	rVB	1200606	2888095	21.40%	5.160%

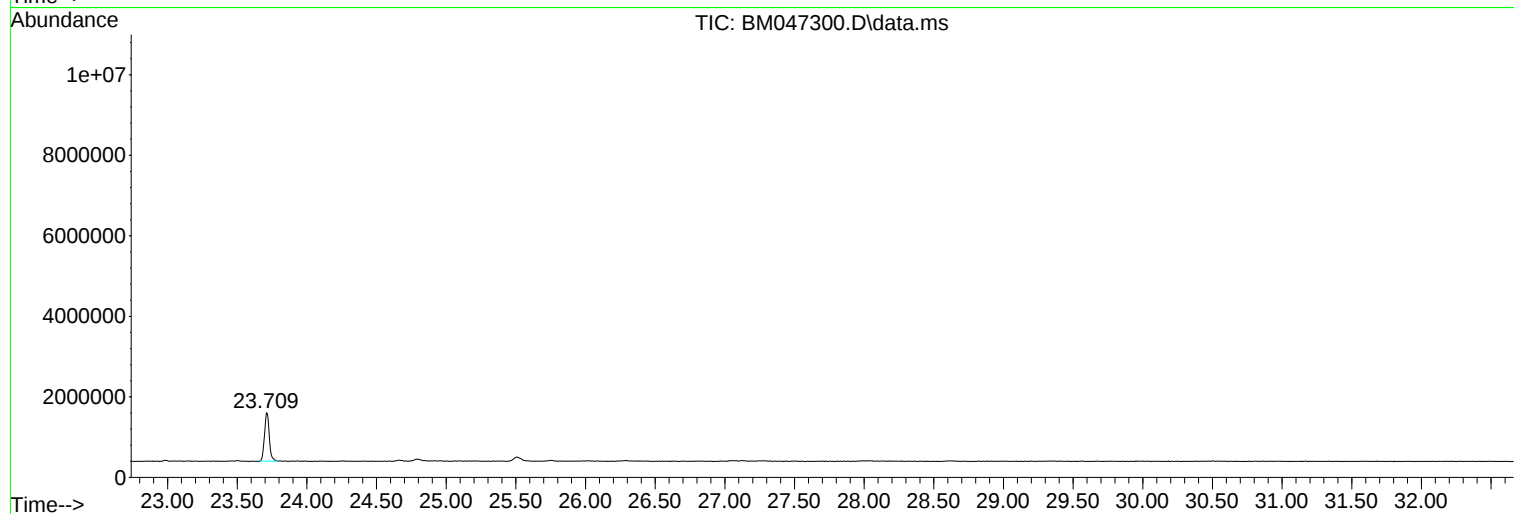
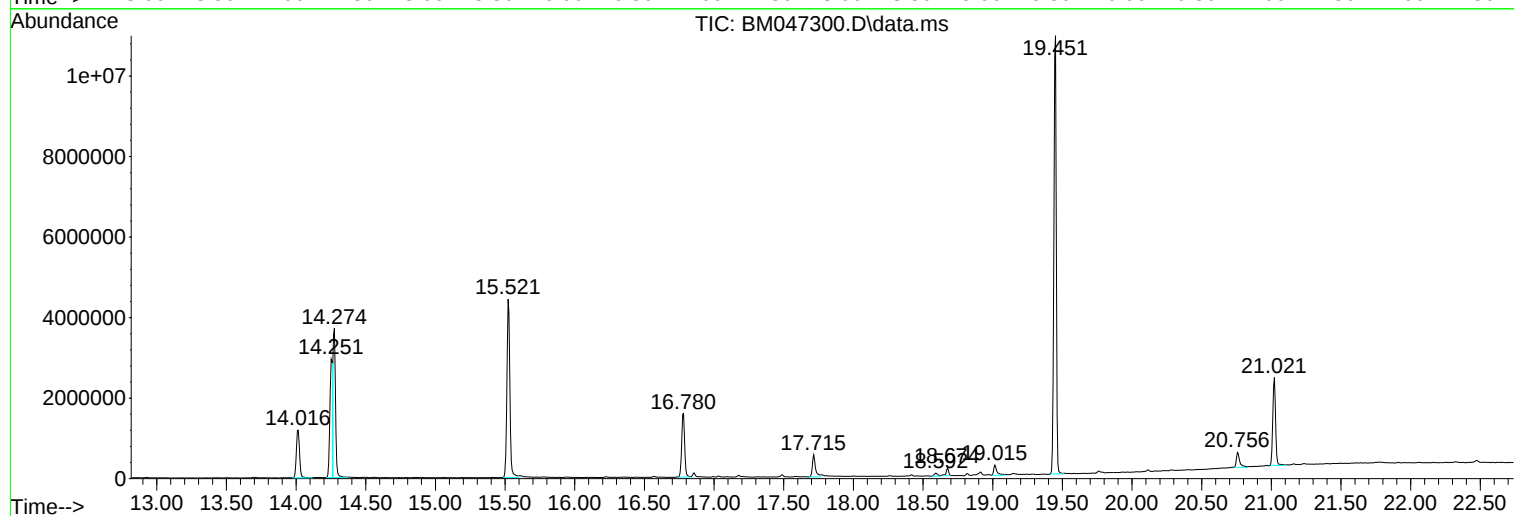
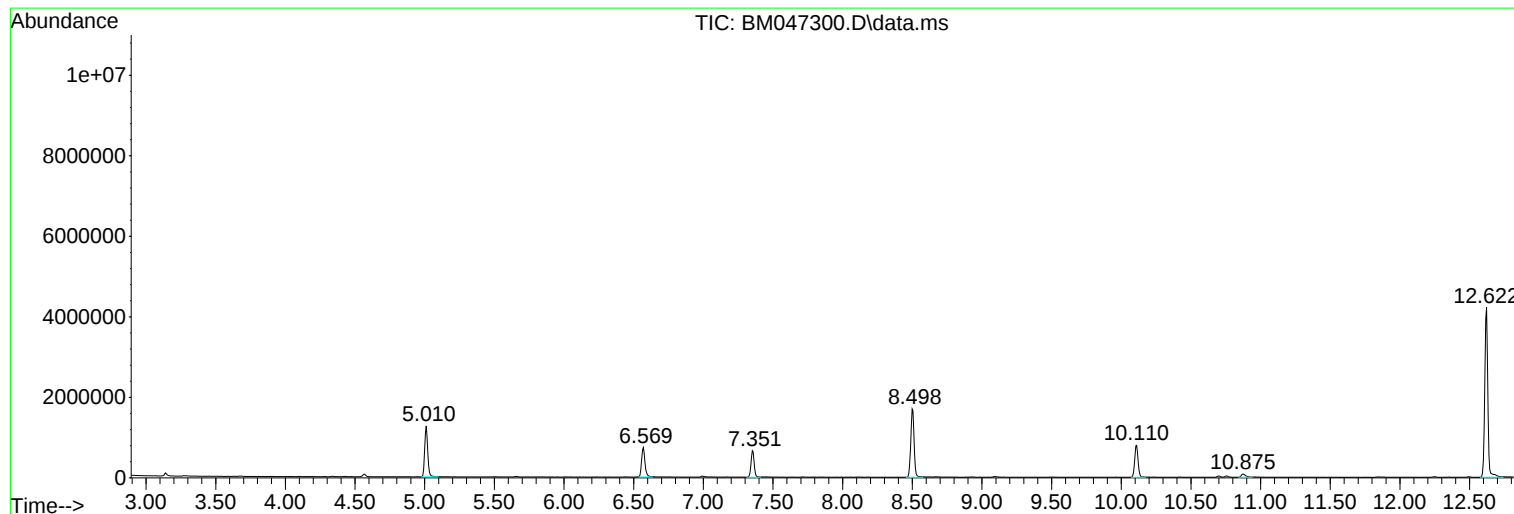
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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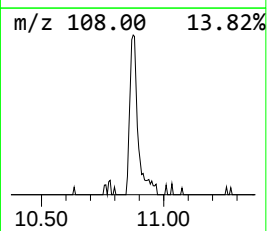
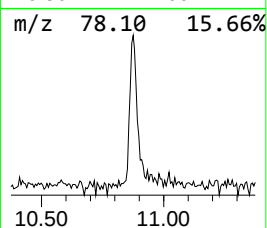
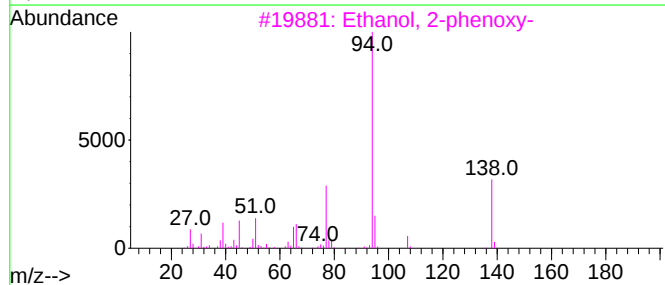
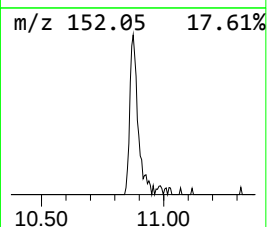
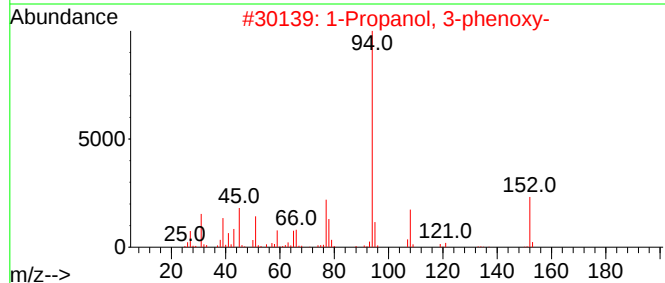
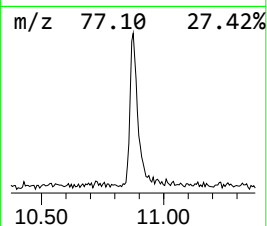
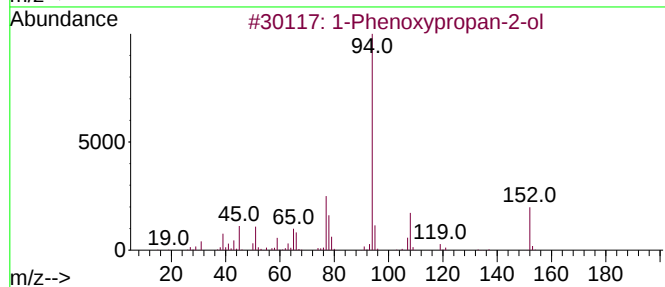
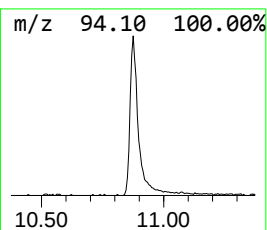
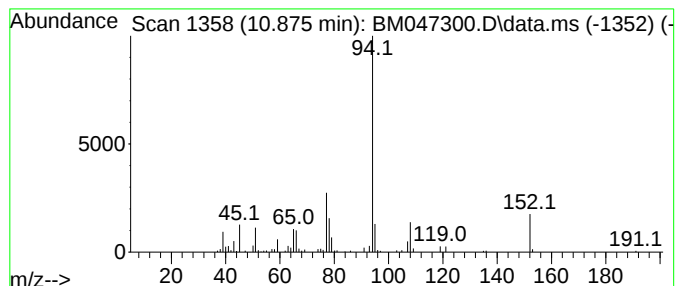
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.875	2.66 ng	180181	Naphthalene-d8	10.110

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
5			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59



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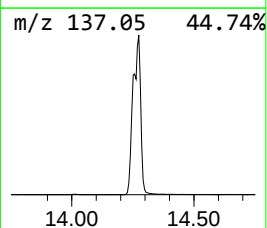
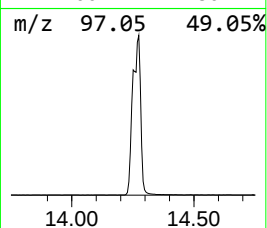
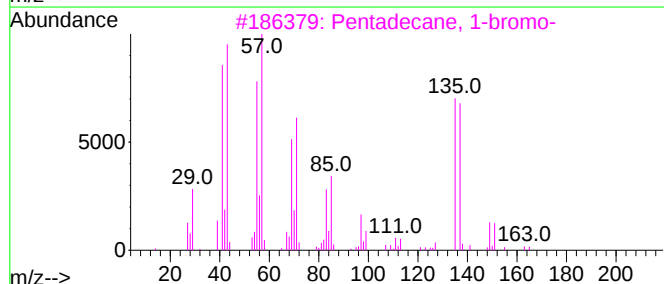
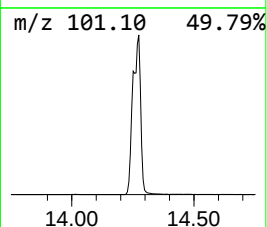
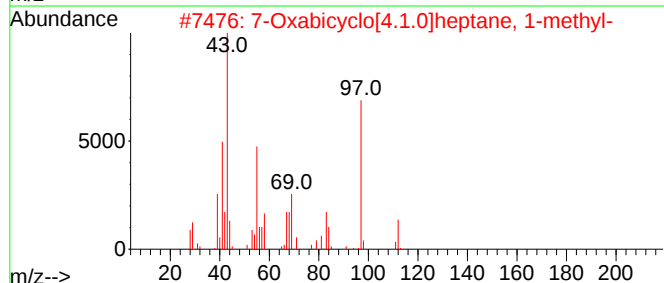
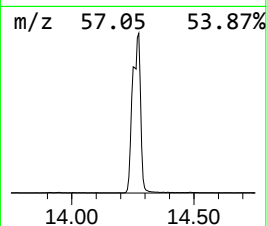
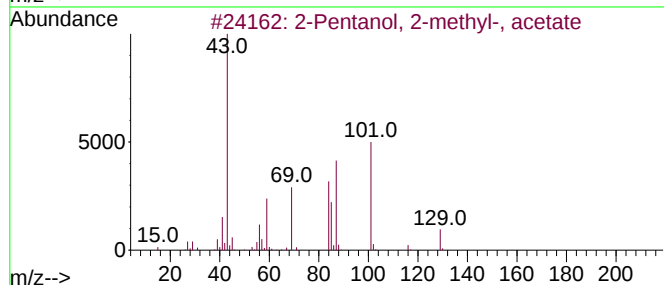
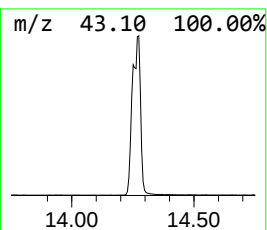
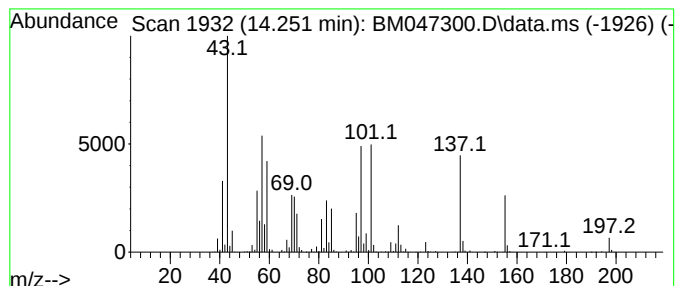
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Peak Number 2 unknown14.251 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.251	46.50 ng	4345250	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	14
2			7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	10
3			Pentadecane, 1-bromo-	290	C15H31Br	000629-72-1	10
4			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	10
5			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	10



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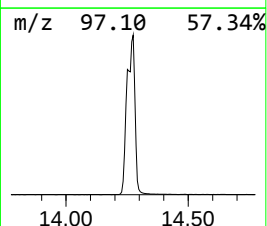
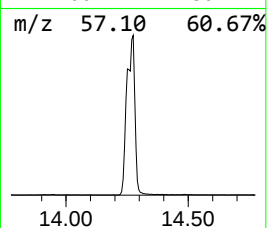
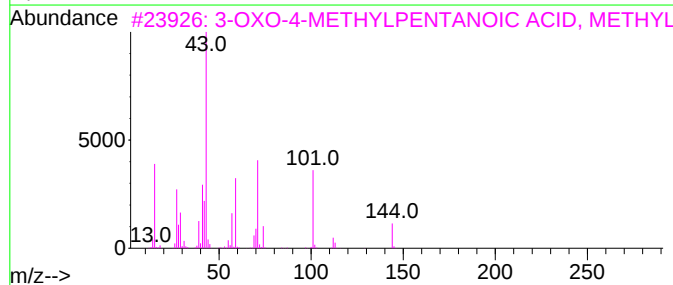
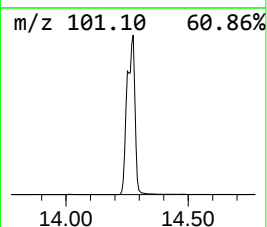
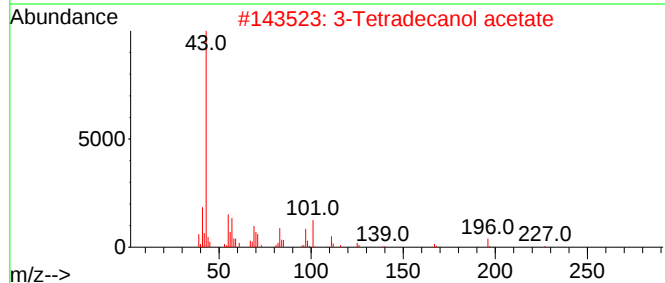
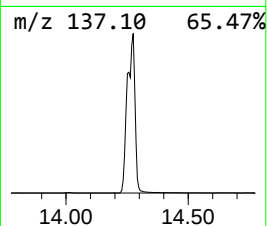
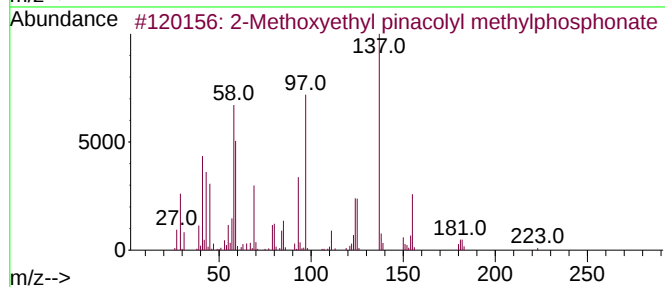
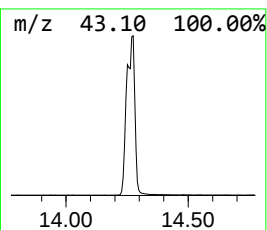
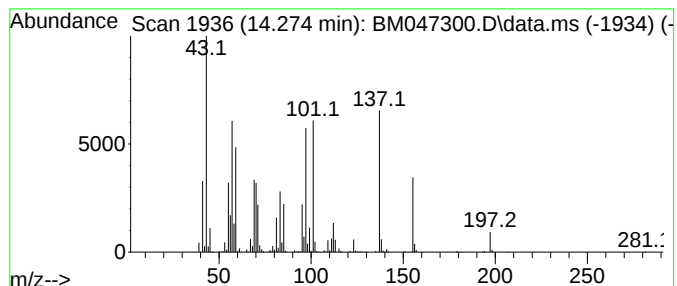
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown14.275 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.275	43.67 ng	4081140	Acenaphthene-d10	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxyethyl pinacolyl methylp...	238	C10H23O4P	177600-27-0	37		
2	3-Tetradecanol acetate	256	C16H32O2	051354-23-5	35		
3	3-OXO-4-METHYLPENTANOIC ACID, ME...	144	C7H12O3	042558-54-3	22		
4	1-(2-Furyl)-3-buten-1-ol	138	C8H10O2	1000311-94-9	11		
5	2,2,3,4-Tetramethylhex-5-en-3-ol	156	C10H20O	1010191-06-9	10		



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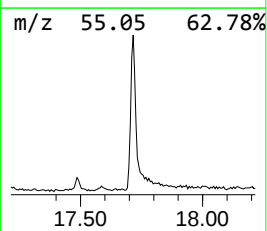
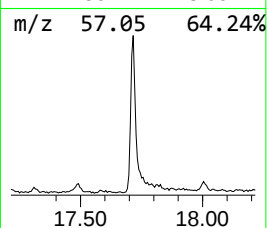
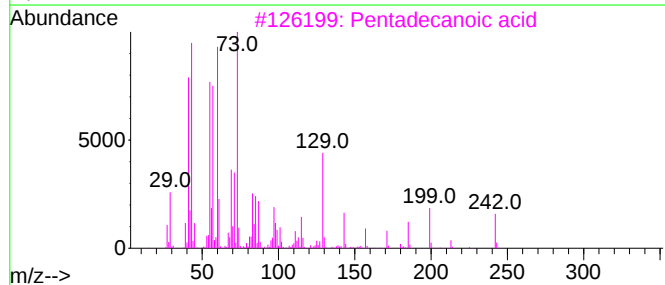
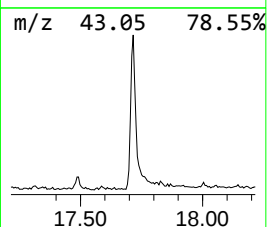
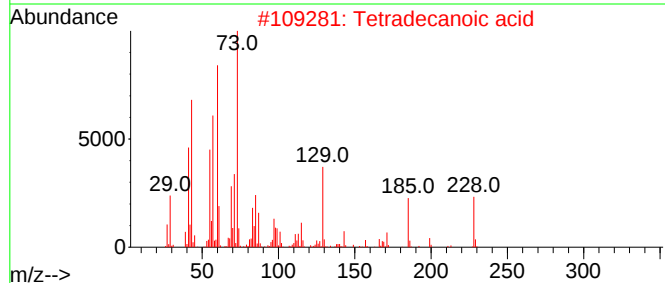
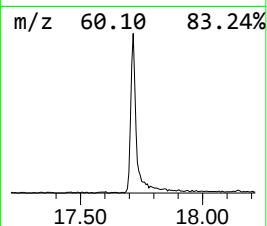
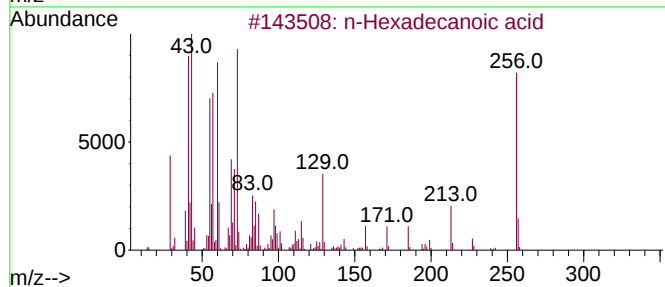
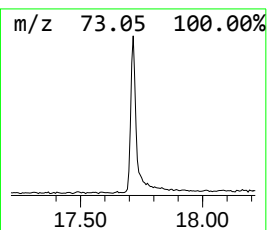
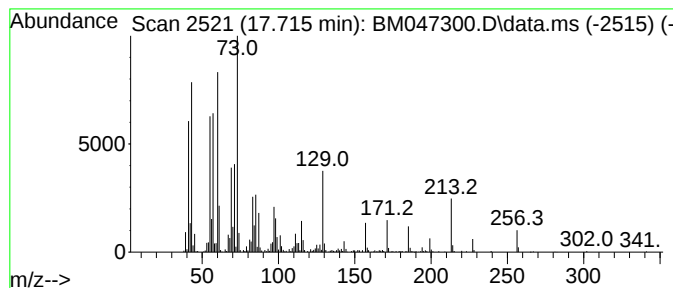
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	7.23 ng	854409	Phenanthrene-d10	16.780

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	91
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Octadecanoic acid	284	C18H36O2	000057-11-4	87
5			Tridecanoic acid	214	C13H26O2	000638-53-9	81



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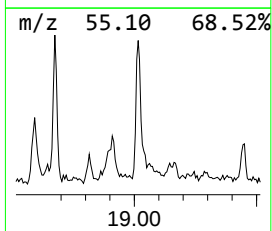
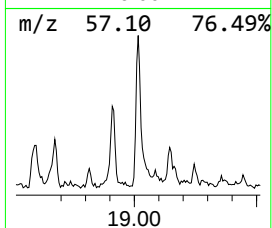
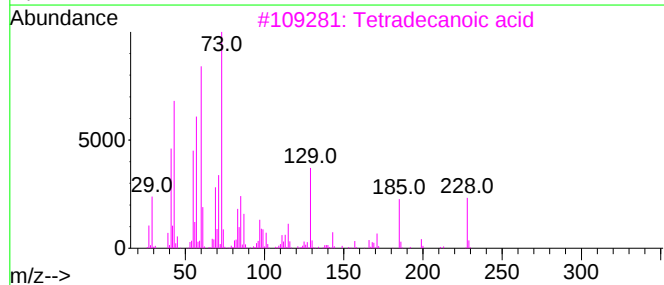
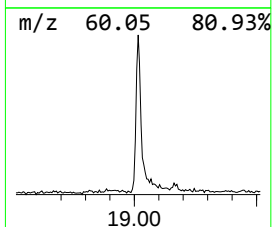
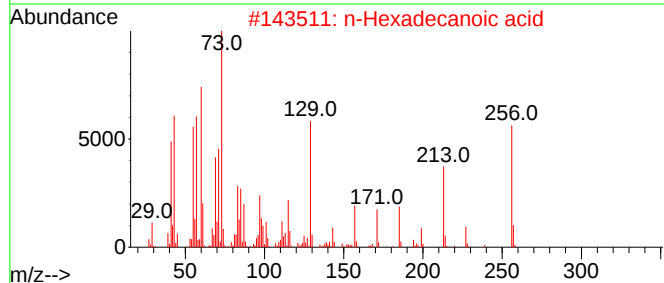
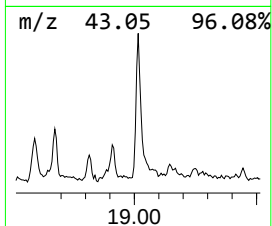
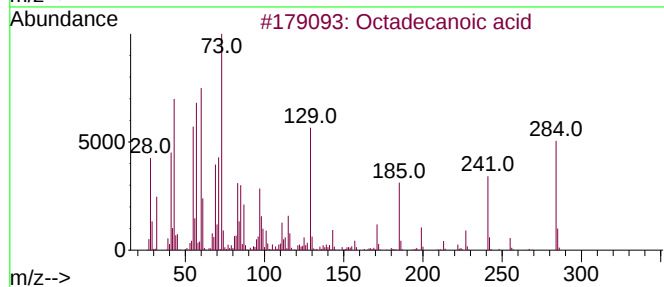
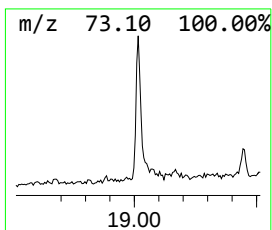
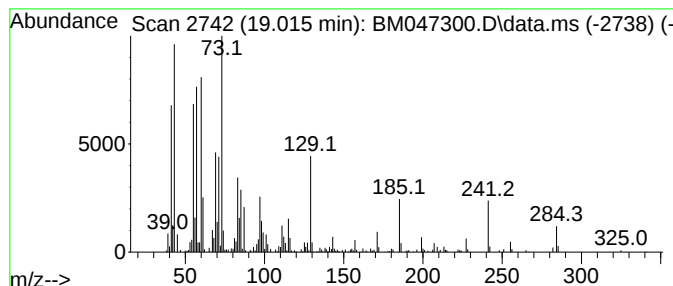
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Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	2.85 ng	424525	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	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			n-Decanoic acid	172	C10H20O2	000334-48-5	70



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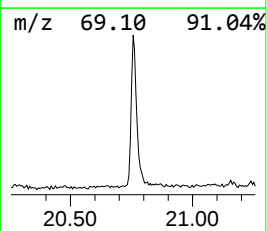
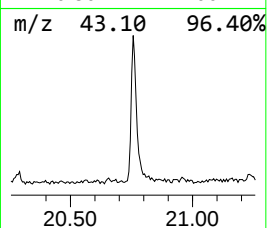
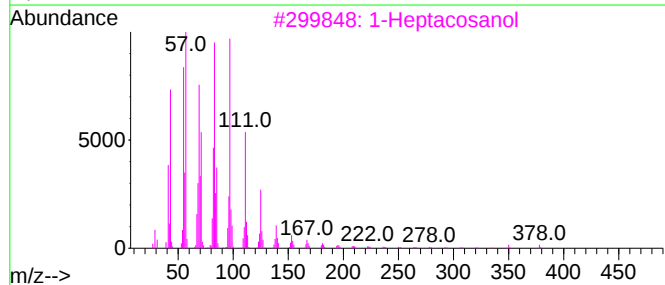
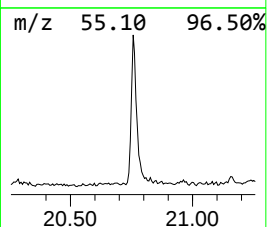
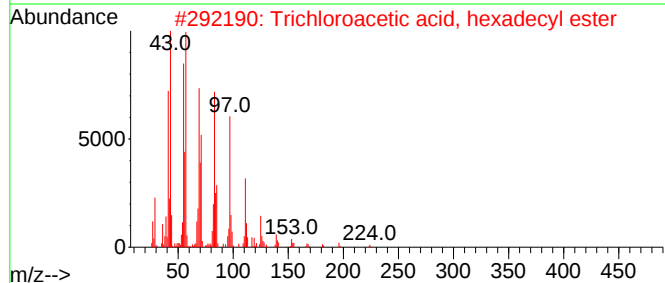
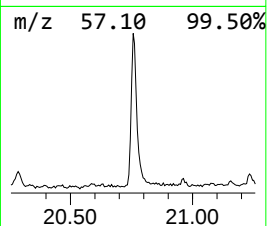
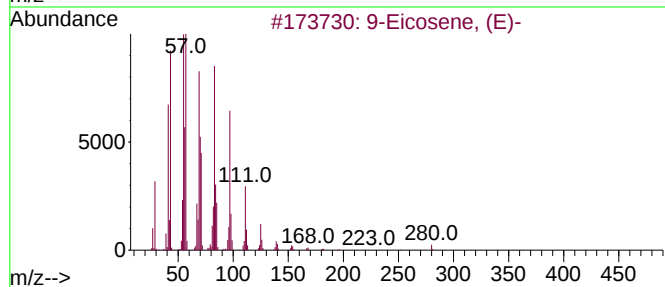
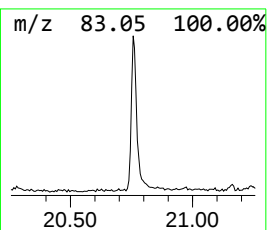
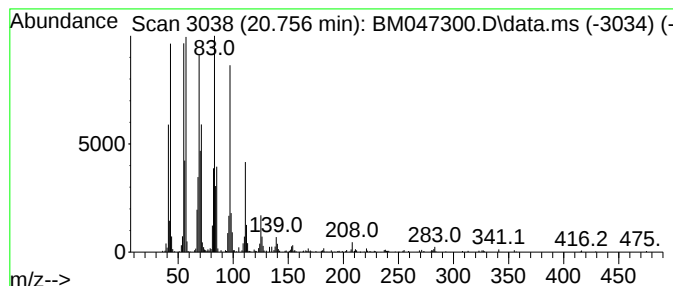
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Eicosene, (E)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.756	4.31 ng	643520	Chrysene-d12	21.021

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Eicosene, (E)-	280	C20H40	074685-29-3	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			1-Heptacosanol	396	C27H56O	002004-39-9	94
4			Behenic alcohol	326	C22H46O	000661-19-8	94
5			1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082124\
Data File : BM047300.D
Acq On : 21 Aug 2024 16:26
Operator : RC/JU
Sample : P3596-01
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
918-J-WS-081324

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM081024.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Phenoxypropan...	10.875	2.7	ng	180181	2	10.110	1352460	20.0
unknown14.251	14.251	46.5	ng	4345250	3	14.010	1868990	20.0
unknown14.275	14.275	43.7	ng	4081140	3	14.010	1868990	20.0
n-Hexadecanoic ...	17.715	7.2	ng	854409	4	16.780	2363680	20.0
Octadecanoic acid	19.015	2.9	ng	424525	5	21.021	2982880	20.0
9-Eicosene, (E)-	20.756	4.3	ng	643520	5	21.021	2982880	20.0