

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021523\
 Data File : BM038748.D
 Acq On : 15 Feb 2023 15:04
 Operator : CG/JU
 Sample : 01537-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TEST-PIT-2-(TP2)-COMP-2

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-BM020123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM038748.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.981	298	305	317	rBV	244377	333355	10.35%	2.224%
2	5.451	379	385	394	rBV	712690	1008201	31.30%	6.727%
3	7.069	652	660	671	rBV	706782	1054295	32.73%	7.035%
4	7.892	794	800	809	rBV	208837	314659	9.77%	2.100%
5	9.069	992	1000	1015	rBV	413995	657357	20.41%	4.386%
6	10.704	1271	1278	1285	rBV	259334	423325	13.14%	2.825%
7	13.163	1689	1696	1703	rBV	1332983	1840369	57.14%	12.280%
8	14.539	1923	1930	1937	rBV	443237	631806	19.62%	4.216%
9	15.898	2154	2161	2167	rBV	75191	101180	3.14%	0.675%
10	16.027	2177	2183	2199	rVB	1247314	1609974	49.99%	10.743%
11	17.280	2390	2396	2401	rBV	569766	756916	23.50%	5.051%
12	18.168	2541	2547	2557	rBV	302986	430161	13.36%	2.870%
13	19.333	2741	2745	2750	rVB	42650	70979	2.20%	0.474%
14	19.439	2759	2763	2778	rBV	137408	213704	6.64%	1.426%
15	19.698	2804	2807	2815	rVB	43141	59394	1.84%	0.396%
16	19.897	2836	2841	2848	rBV	2721983	3220857	100.00%	21.492%
17	20.445	2931	2934	2940	rBV	44694	57406	1.78%	0.383%
18	21.150	3050	3054	3066	rBV	179712	277797	8.62%	1.854%
19	21.462	3101	3107	3111	rBV	723139	965559	29.98%	6.443%
20	23.838	3505	3511	3521	rVB2	497794	959159	29.78%	6.400%

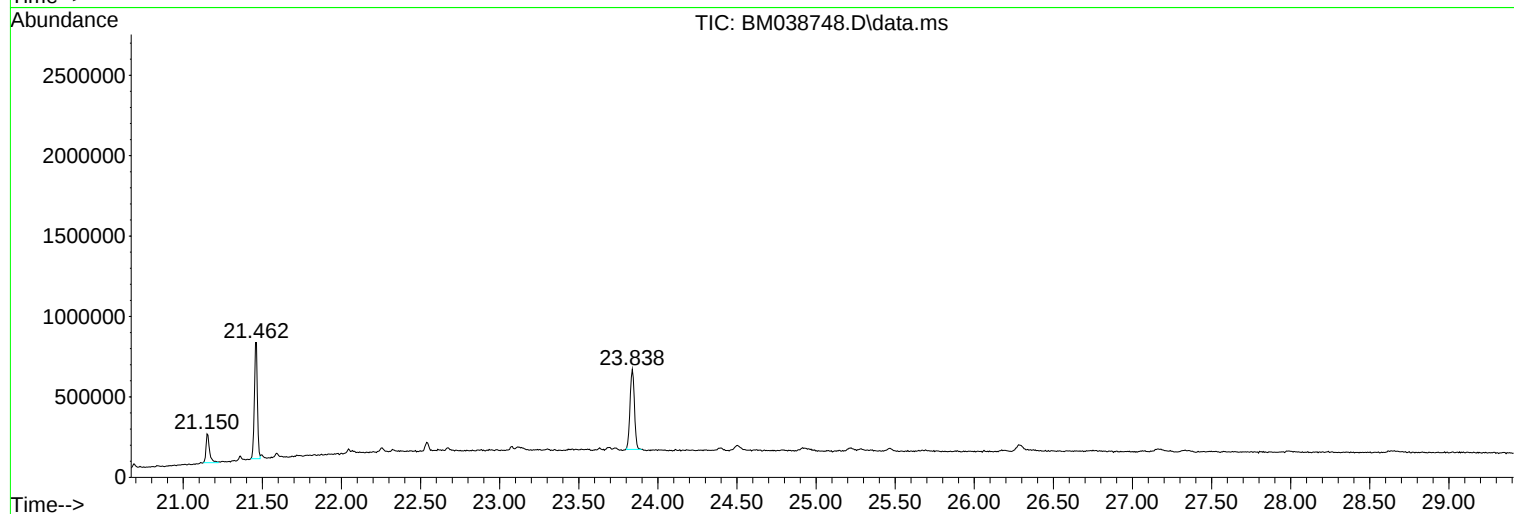
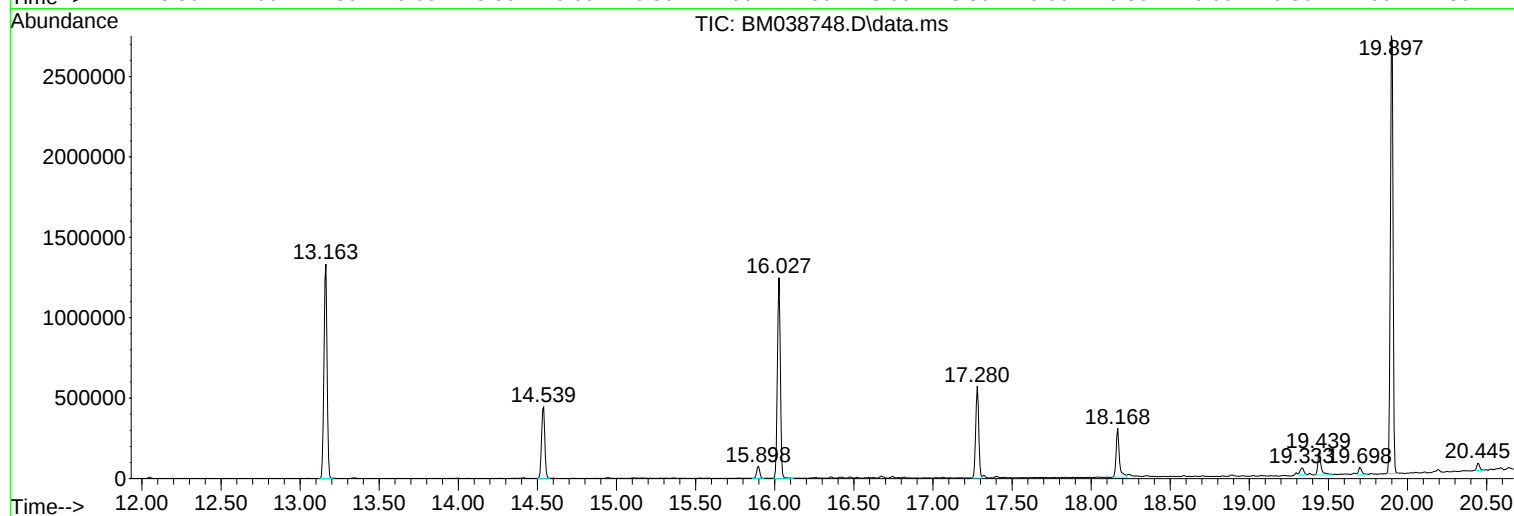
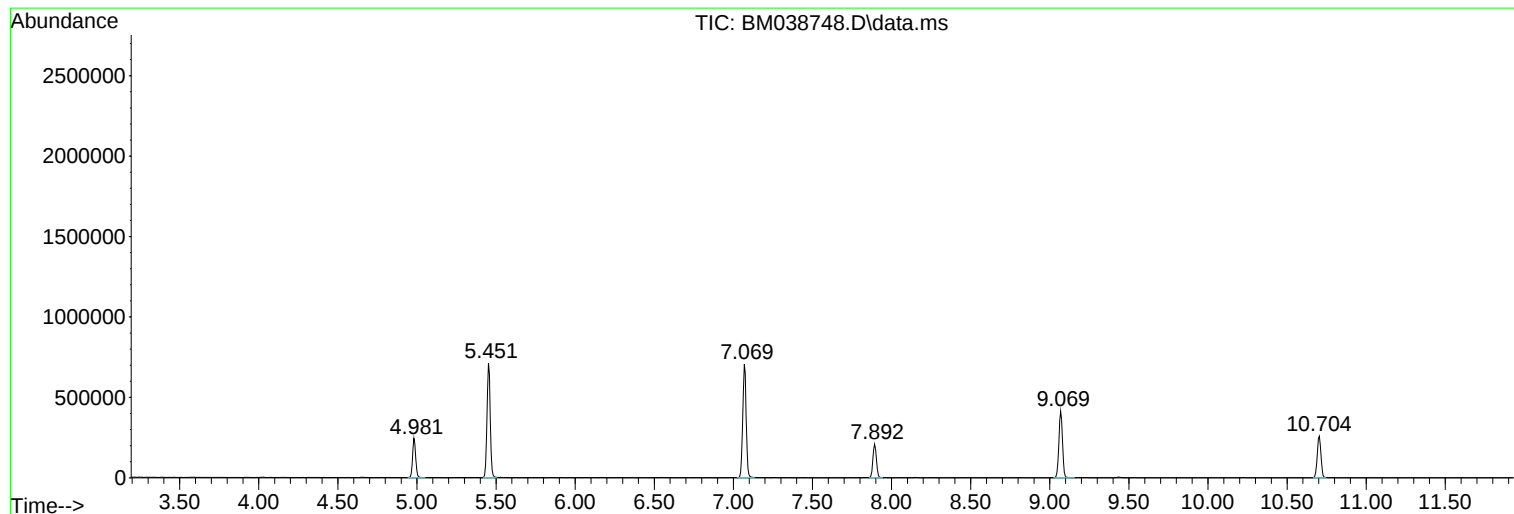
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
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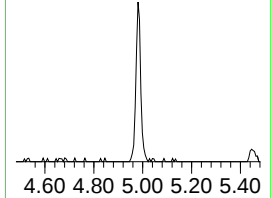
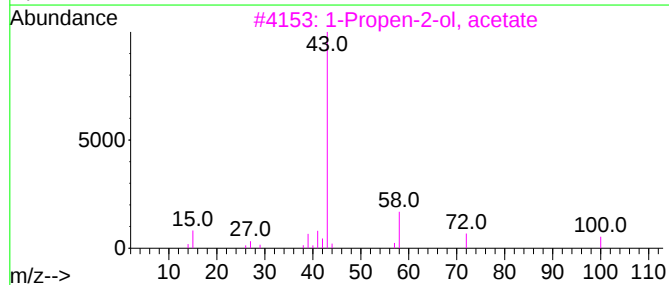
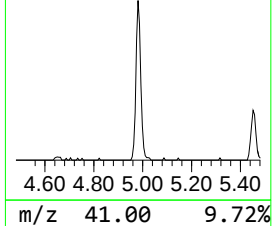
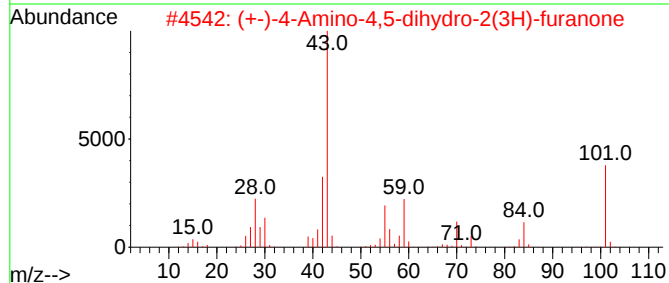
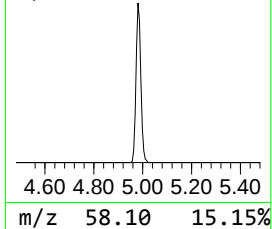
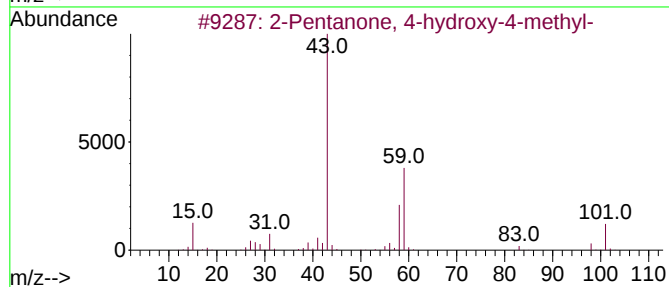
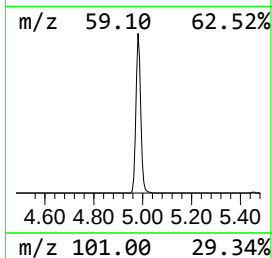
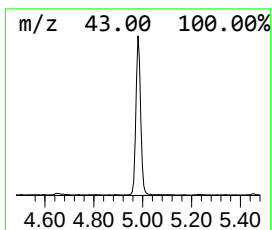
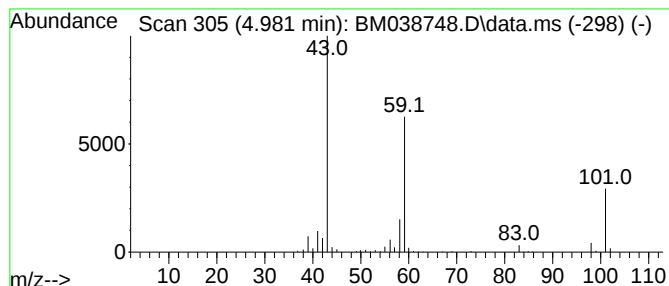
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.981	21.19 ng	333355	1,4-Dichlorobenzene-d4	7.892

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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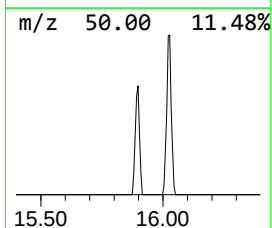
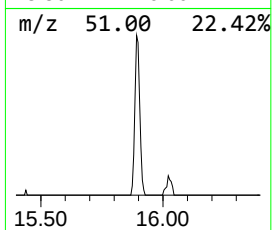
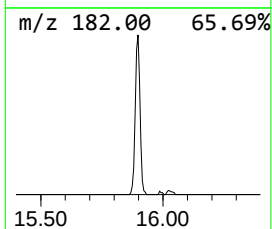
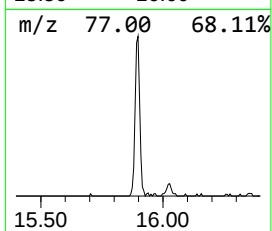
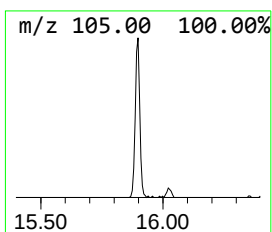
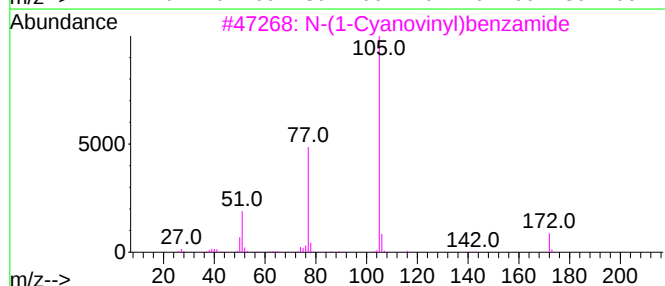
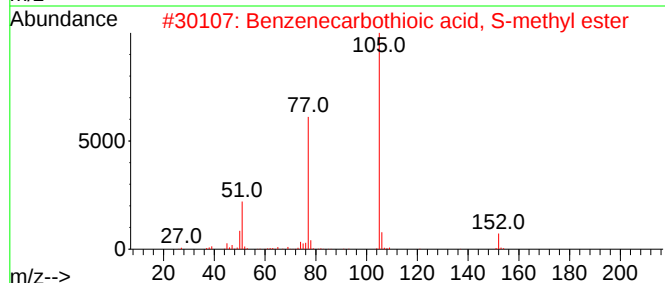
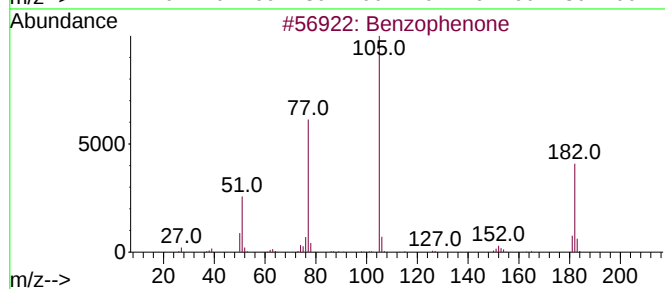
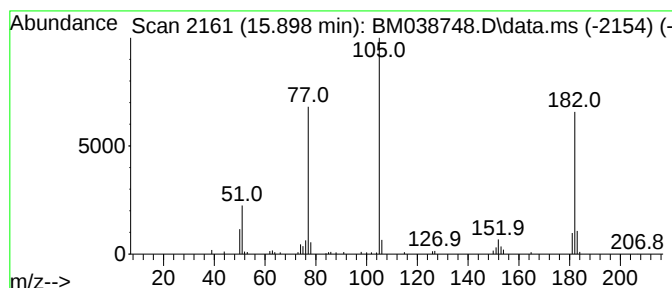
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Peak Number 2 Benzophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	3.20 ng	101180	Acenaphthene-d10	14.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	95
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	46
3			N-(1-Cyanovinyl)benzamide	172	C10H8N2O	1000186-19-1	38
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	38
5			Ethanedione, diphenyl-	210	C14H10O2	000134-81-6	38



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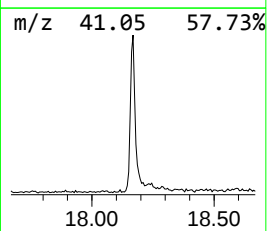
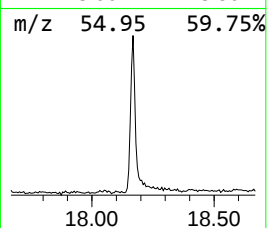
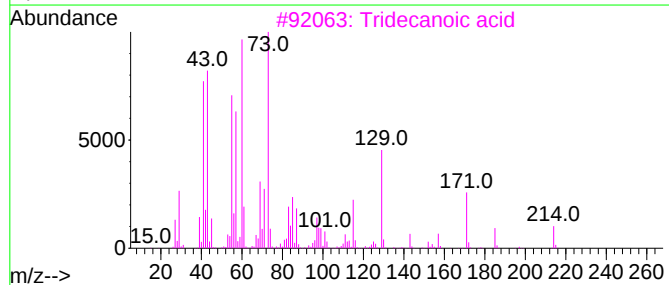
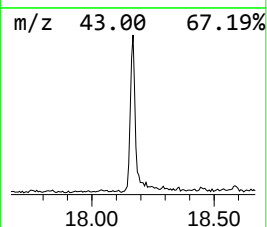
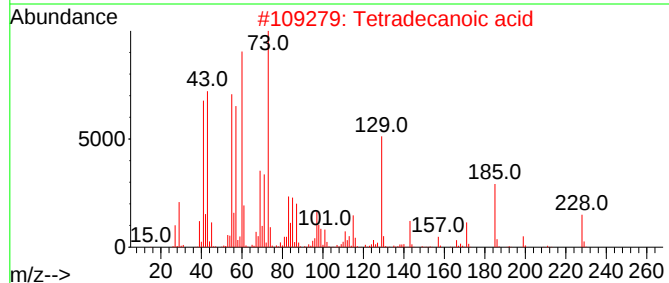
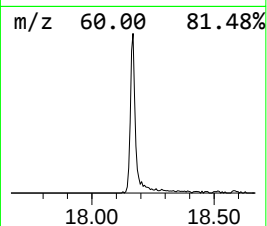
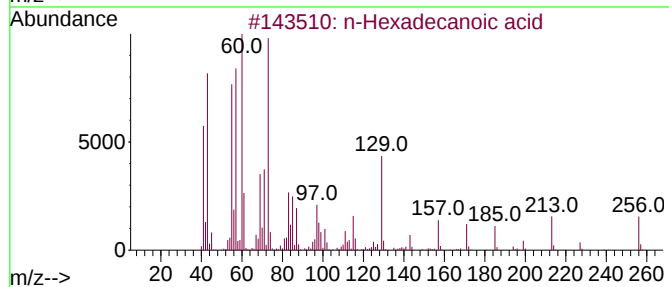
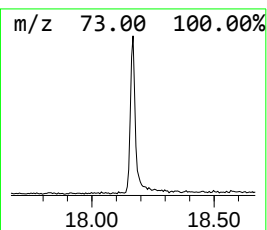
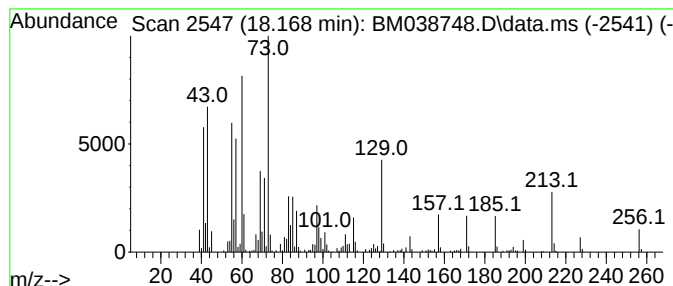
Instrument :
BNA_M
ClientSampleId :
TEST-PIT-2-(TP2)-COMP-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM020123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.168	11.37 ng	430161	Phenanthrene-d10		17.280	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	98
2	Tetradecanoic acid		228	C14H28O2	000544-63-8	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	89
4	Undecanoic acid		186	C11H22O2	000112-37-8	76
5	Pentadecanoic acid		242	C15H30O2	001002-84-2	68



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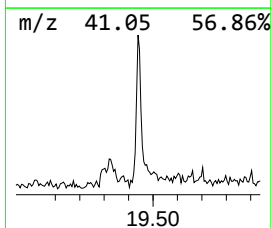
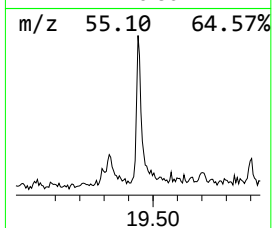
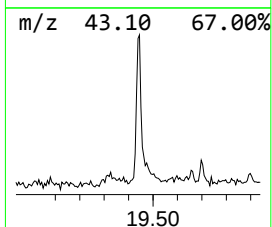
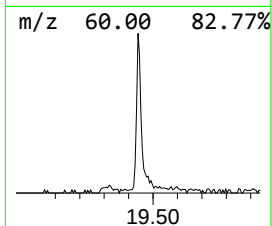
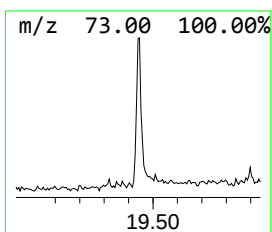
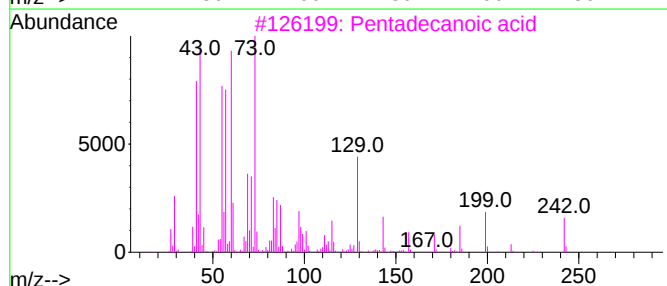
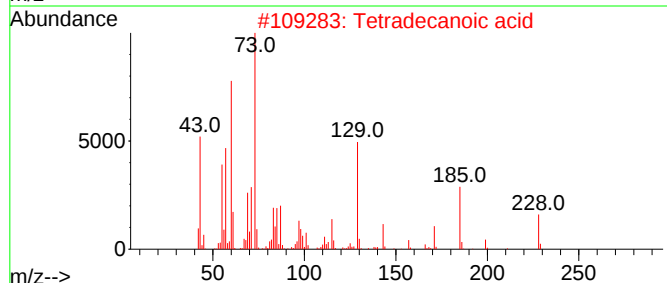
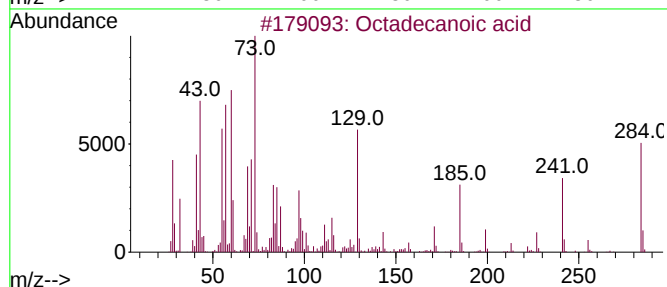
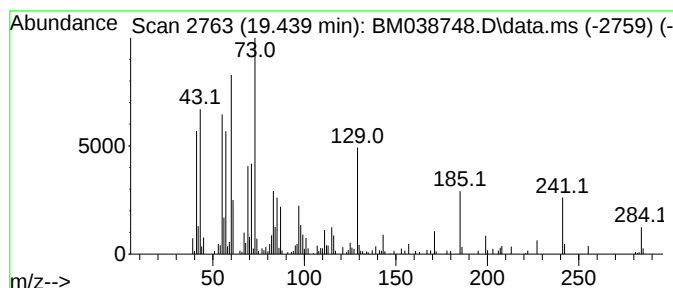
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	4.43 ng	213704	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	72



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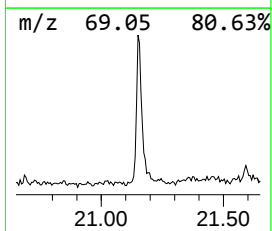
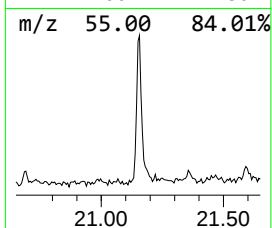
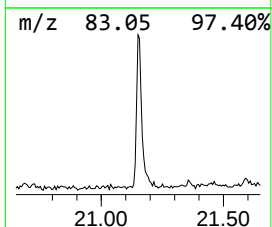
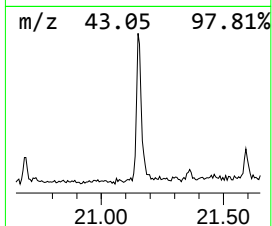
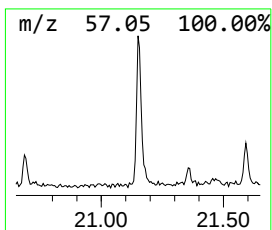
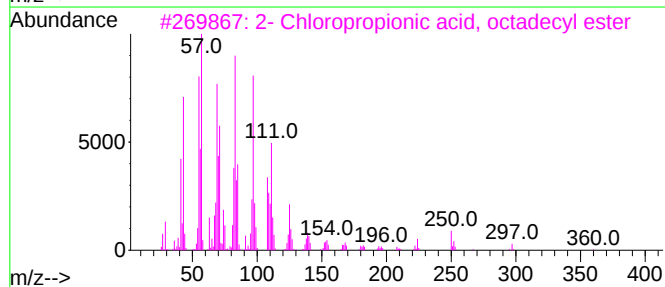
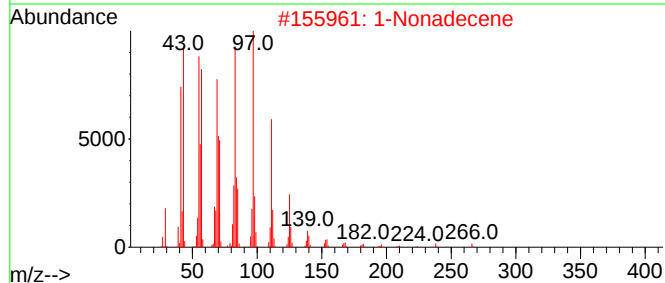
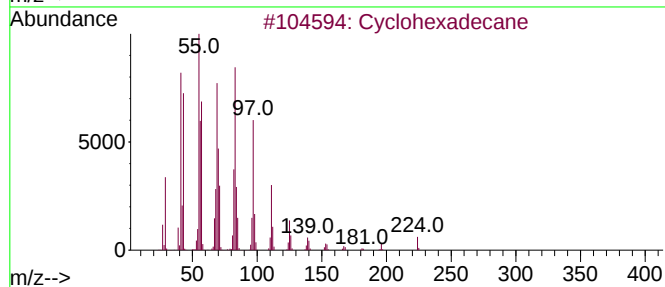
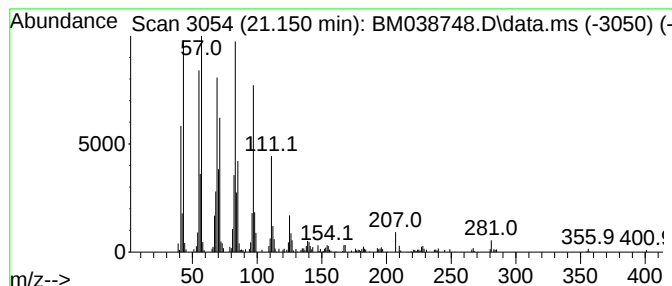
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.150	5.75 ng	277797	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	99
2			1-Nonadecene	266	C19H38	018435-45-5	96
3			2- Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	94
4			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	93
5			1-Hexacosene	364	C26H52	018835-33-1	93



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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
2-Pentanone, 4-...	4.981	21.2	ng	333355	1	7.892	314659	20.0
Benzophenone	15.898	3.2	ng	101180	3	14.539	631806	20.0
n-Hexadecanoic ...	18.168	11.4	ng	430161	4	17.280	756916	20.0
Octadecanoic acid	19.439	4.4	ng	213704	5	21.462	965559	20.0
Cyclohexadecane	21.150	5.8	ng	277797	5	21.462	965559	20.0