

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
 Data File : BM038734.D
 Acq On : 14 Feb 2023 17:33
 Operator : CG/JU
 Sample : 01329-16
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 COMP-9-BORING-2-28-35

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: BM038734.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.987	300	306	314	rBV	203878	271031	18.17%	3.085%
2	5.457	380	386	395	rBV	581203	800318	53.67%	9.109%
3	7.075	655	661	675	rBV	523800	789603	52.95%	8.987%
4	7.898	795	801	808	rBV	154877	233572	15.66%	2.658%
5	9.075	993	1001	1013	rBV	302447	476838	31.97%	5.427%
6	10.710	1272	1279	1288	rVB	167513	275132	18.45%	3.131%
7	13.163	1690	1696	1703	rBV	831962	1151760	77.23%	13.109%
8	14.539	1924	1930	1943	rVB	260734	379118	25.42%	4.315%
9	15.898	2156	2161	2166	rBV	28636	37998	2.55%	0.432%
10	16.027	2178	2183	2197	rBV	699327	964282	64.66%	10.975%
11	17.286	2391	2397	2408	rBV	300047	419363	28.12%	4.773%
12	18.168	2542	2547	2558	rBV	90745	134889	9.05%	1.535%
13	19.445	2759	2764	2774	rBV	33842	58653	3.93%	0.668%
14	19.721	2804	2811	2820	rBV	14395	32665	2.19%	0.372%
15	19.903	2836	2842	2848	rBV	1310698	1491286	100.00%	16.973%
16	21.156	3051	3055	3061	rBV3	66478	94573	6.34%	1.076%
17	21.462	3102	3107	3114	rBV	418810	503366	33.75%	5.729%
18	22.327	3252	3254	3259	rVB3	47899	55883	3.75%	0.636%
19	23.844	3506	3512	3519	rVB2	311030	615637	41.28%	7.007%

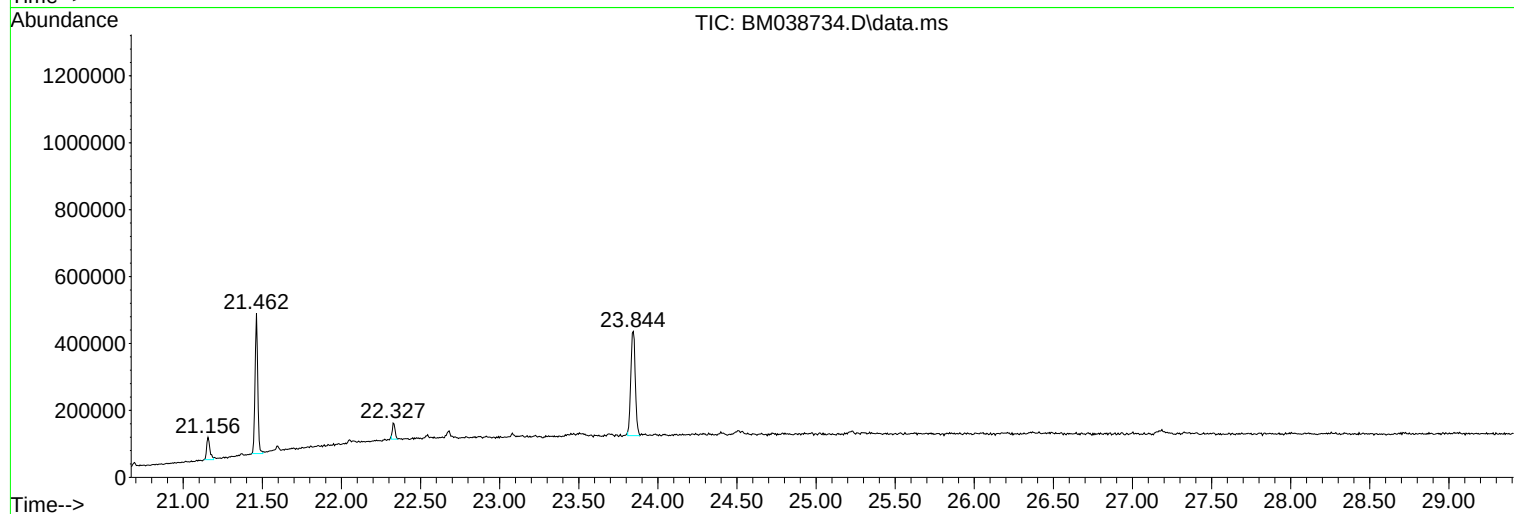
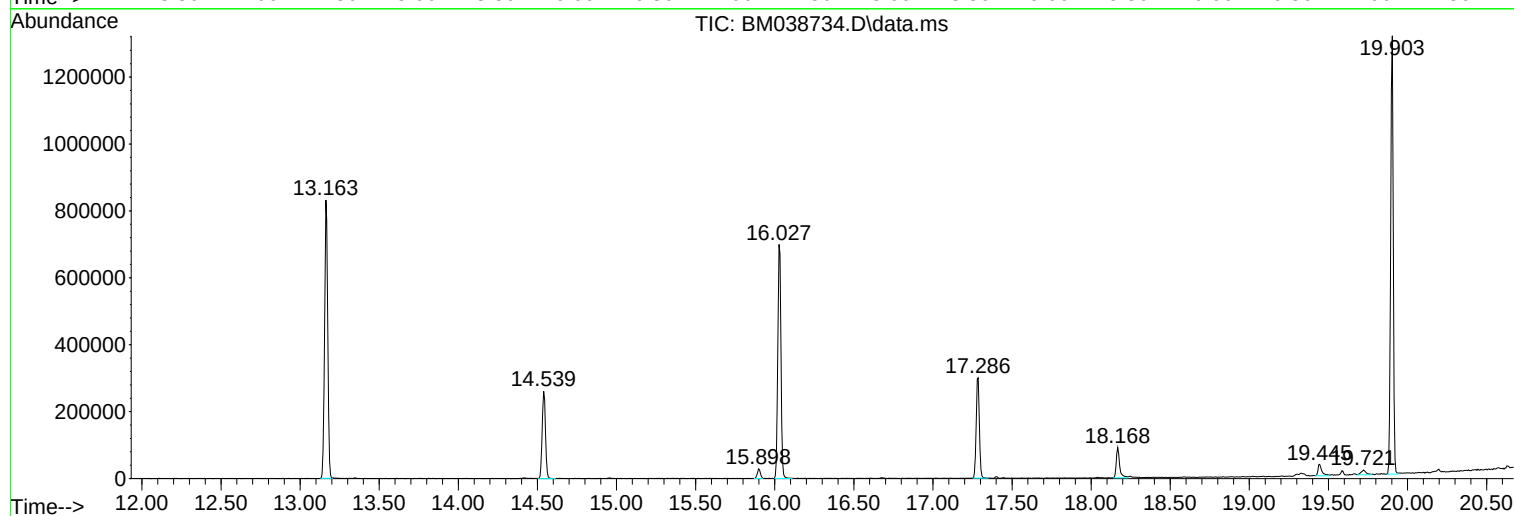
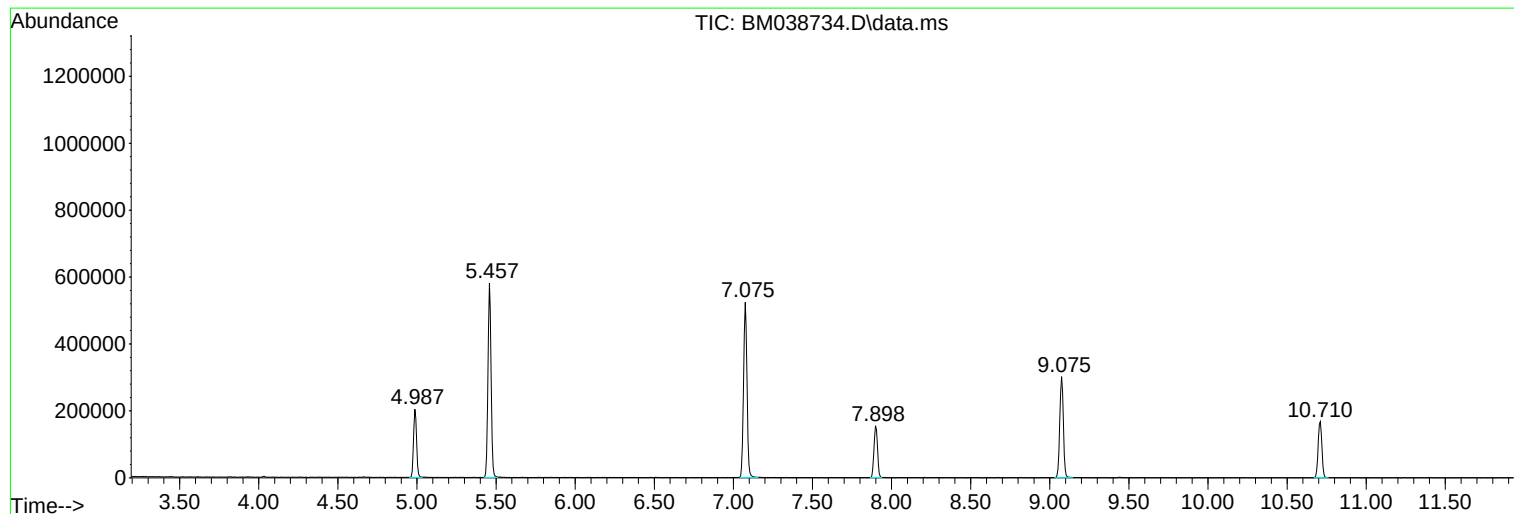
Sum of corrected areas: 8785967

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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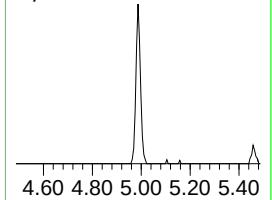
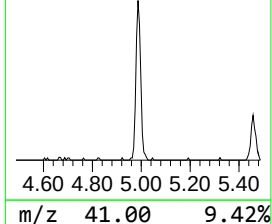
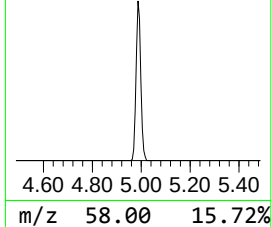
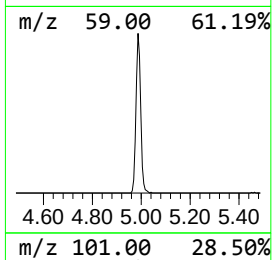
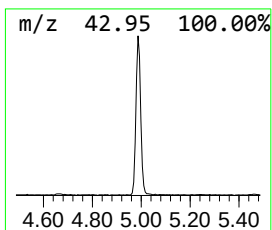
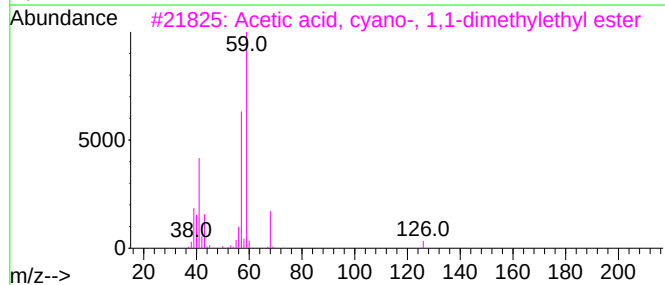
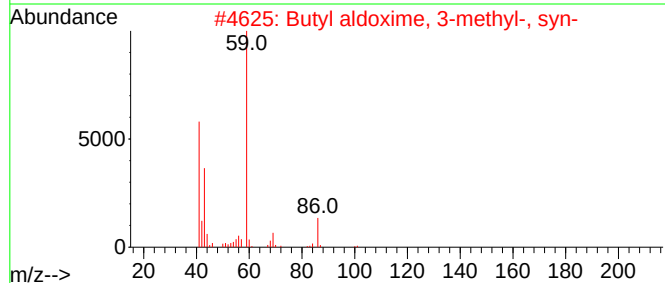
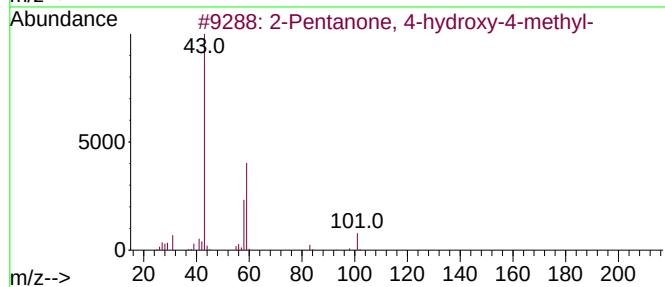
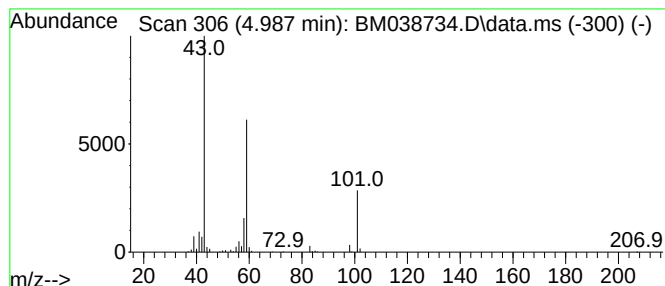
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.987	23.21 ng	271031	1,4-Dichlorobenzene-d4	7.898

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	25		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	4-Methoxy-1-pentene	100	C6H12O	098386-09-5	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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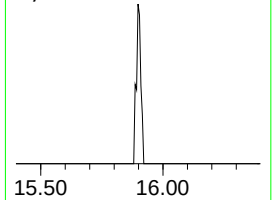
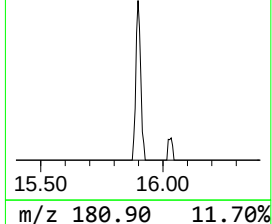
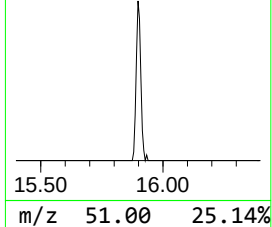
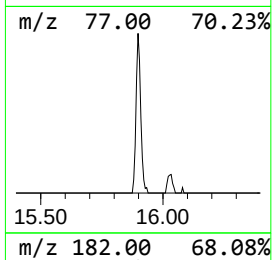
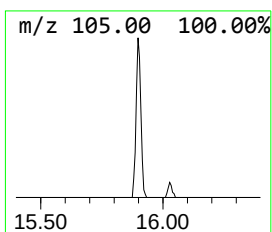
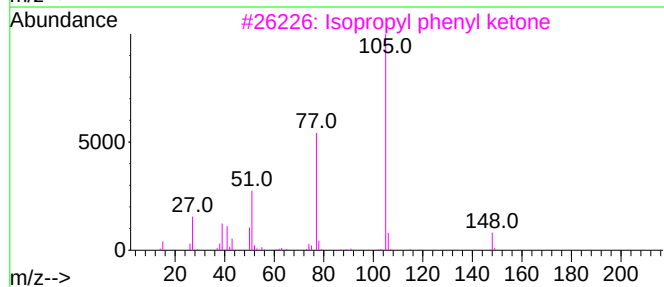
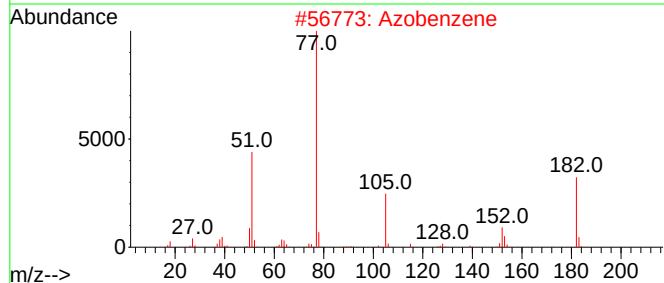
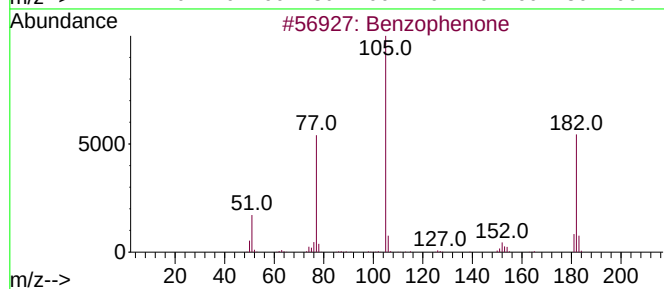
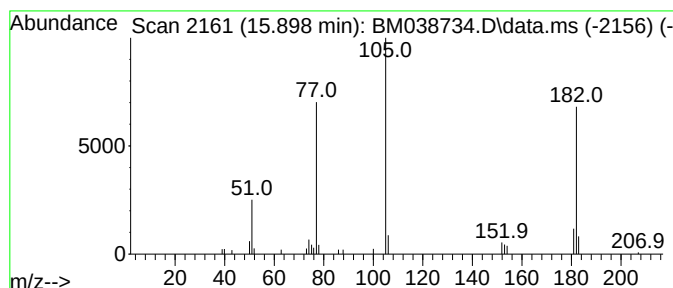
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Peak Number 2 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.898	2.00 ng	37998	Acenaphthene-d10	14.539

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	94
2			Azobenzene	182	C12H10N2	000103-33-3	47
3			Isopropyl phenyl ketone	148	C10H12O	000611-70-1	43
4			3,8-Dibenzoyl-1-nitro-3,6,8-tria...	394	C21H22N4O4	162710-50-1	43
5			Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	43



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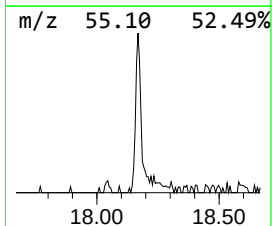
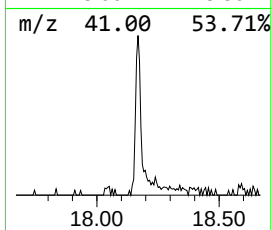
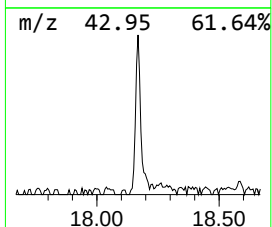
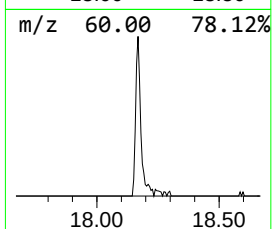
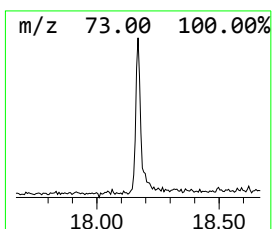
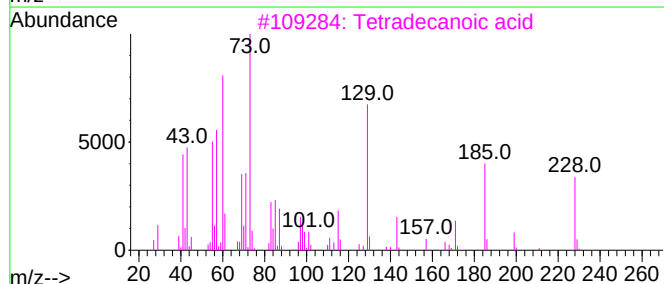
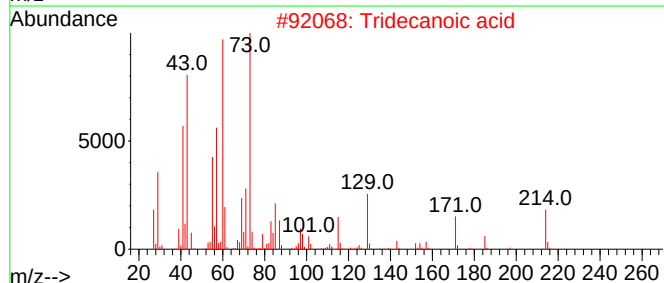
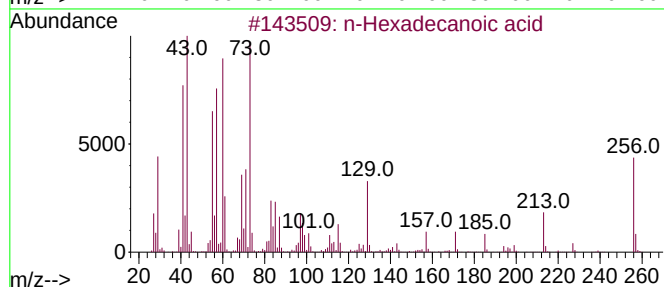
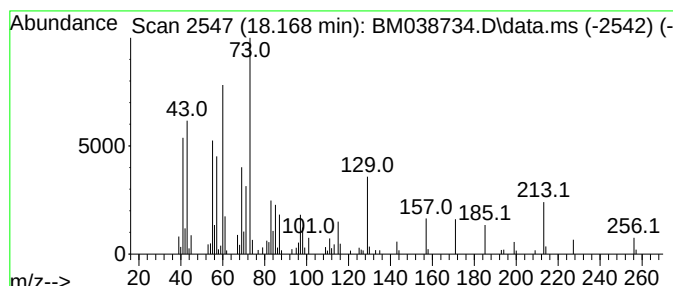
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.168	6.43 ng	134889	Phenanthrene-d10	17.286	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	93
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5	Dodecanoic acid	200	C12H24O2	000143-07-7	53



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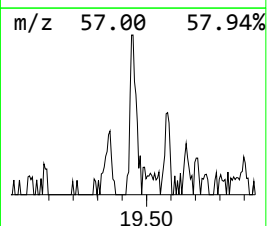
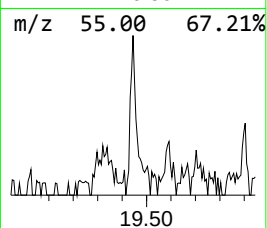
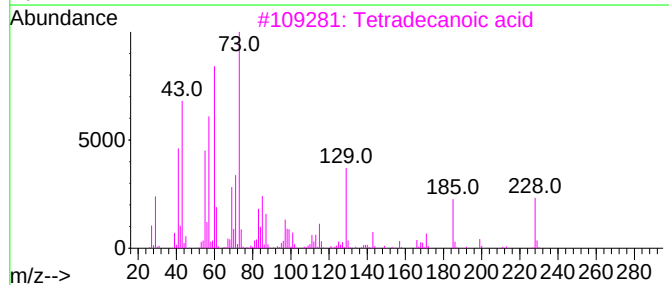
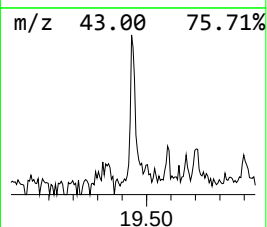
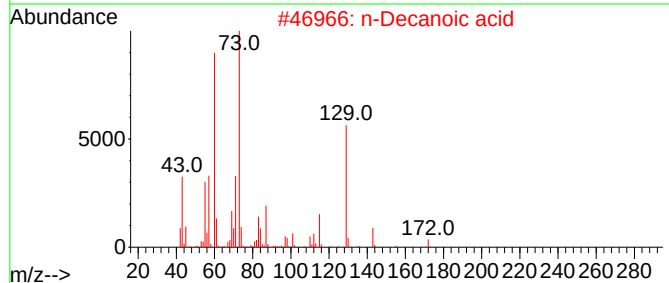
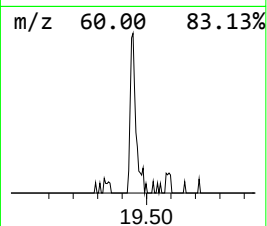
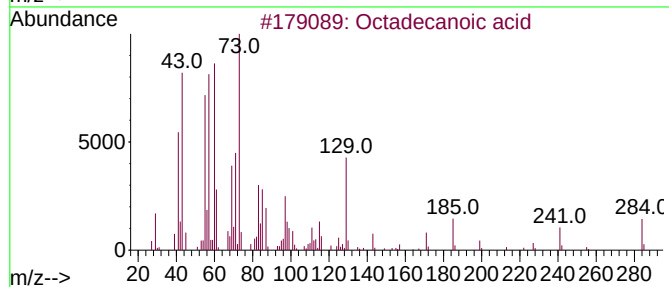
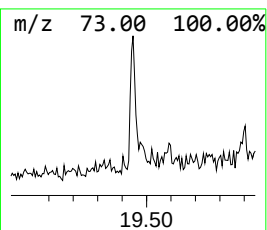
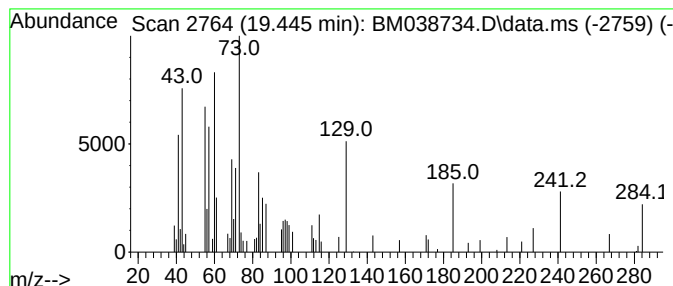
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Peak Number 4 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	2.33 ng	58653	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	93
2			n-Decanoic acid	172	C10H20O2	000334-48-5	92
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	47



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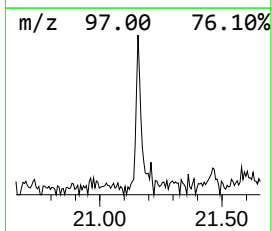
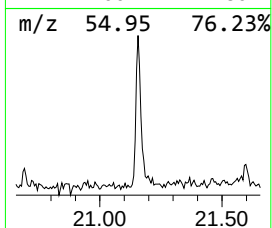
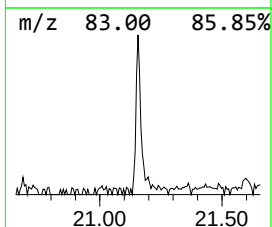
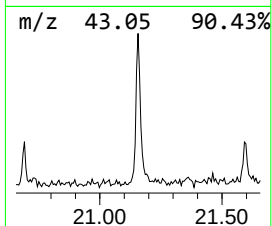
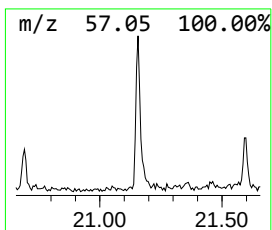
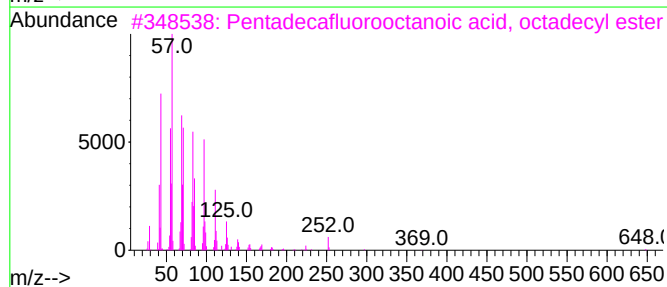
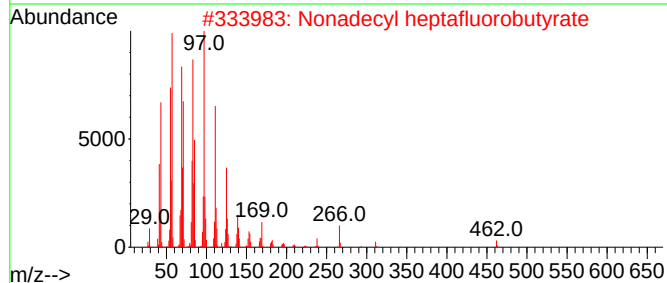
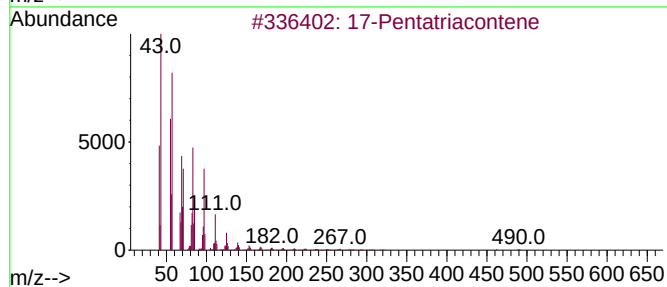
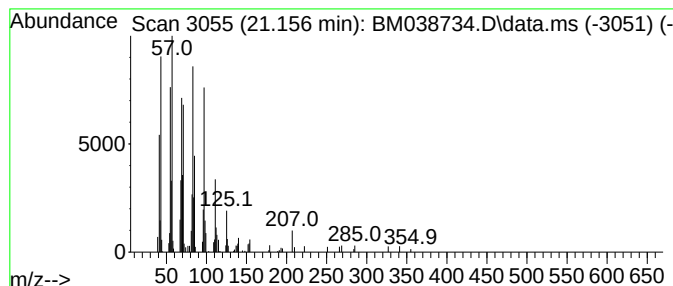
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Peak Number 5 17-Pentatriacontene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.156	3.76 ng	94573	Chrysene-d12	21.462

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			Nonadecyl heptafluorobutyrate	480	C23H39F7O2	1000351-83-9	91
3			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	90
4			Pentacos-1-ene	350	C25H50	016980-85-1	87
5			1-Nonadecene	266	C19H38	018435-45-5	83



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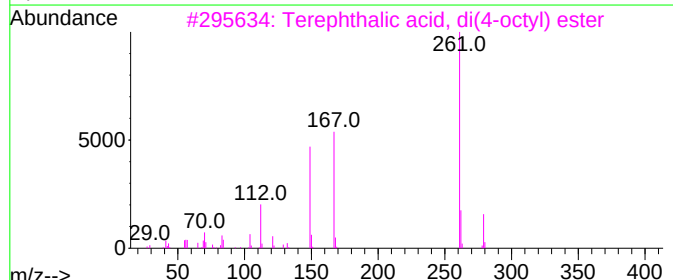
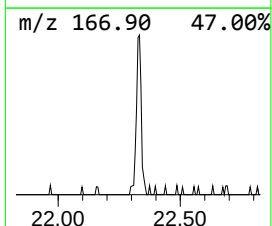
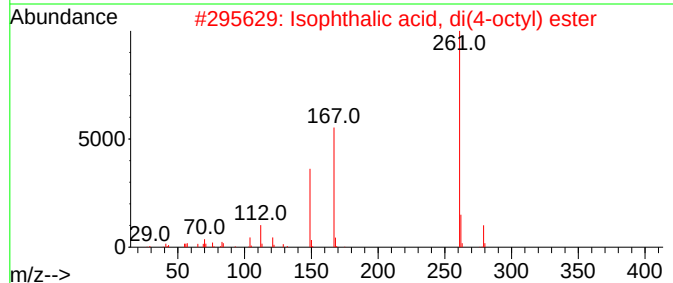
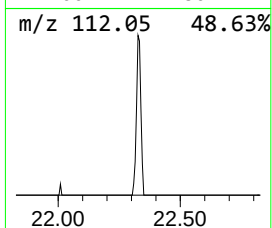
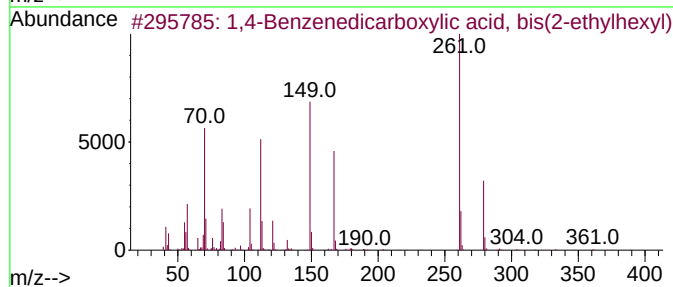
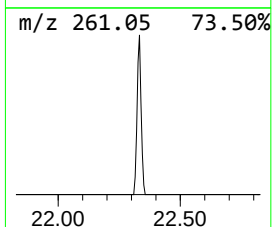
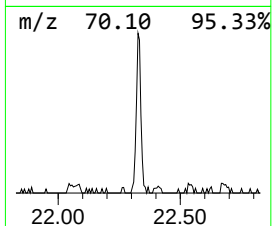
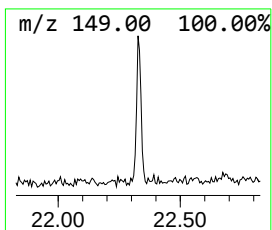
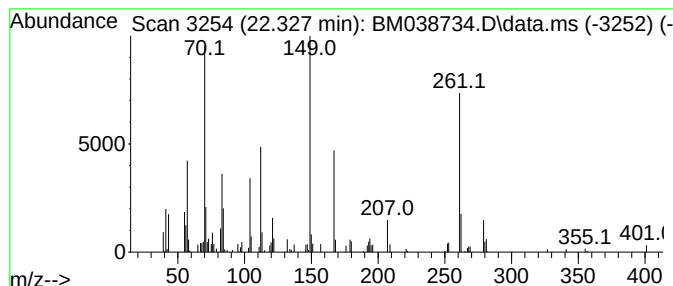
Instrument :
BNA_M
ClientSampleId :
COMP-9-BORING-2-28-35

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
22.327	2.22 ng	55883	Chrysene-d12		21.462	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	1,4-Benzenedicarboxylic acid, bi...		390	C24H38O4	006422-86-2	72
2	Isophthalic acid, di(4-octyl) ester		390	C24H38O4	1000344-04-3	43
3	Terephthalic acid, di(4-octyl) e...		390	C24H38O4	1000323-74-2	43
4	Terephthalic acid, 3-methylbut-2...		348	C21H32O4	1000356-27-6	27
5	6H-Thieno[2,3-b]pyrrole-5-carbox...		167	C7H5NO2S	051856-25-8	18



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM021423\
Data File : BM038734.D
Acq On : 14 Feb 2023 17:33
Operator : CG/JU
Sample : 01329-16
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
COMP-9-BORING-2-28-35

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

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	23.2	ng	271031	1	7.898	233572	20.0
Benzophenone	15.898	2.0	ng	37998	3	14.539	379118	20.0
n-Hexadecanoic ...	18.168	6.4	ng	134889	4	17.286	419363	20.0
Octadecanoic acid	19.445	2.3	ng	58653	5	21.462	503366	20.0
17-Pentatriacon...	21.156	3.8	ng	94573	5	21.462	503366	20.0
1,4-Benzenedica...	22.327	2.2	ng	55883	5	21.462	503366	20.0