

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
 Data File : BM039282.D
 Acq On : 03 Apr 2023 16:58
 Operator : CG/JU
 Sample : 02154-01
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

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-BM032923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM039282.D\data.ms

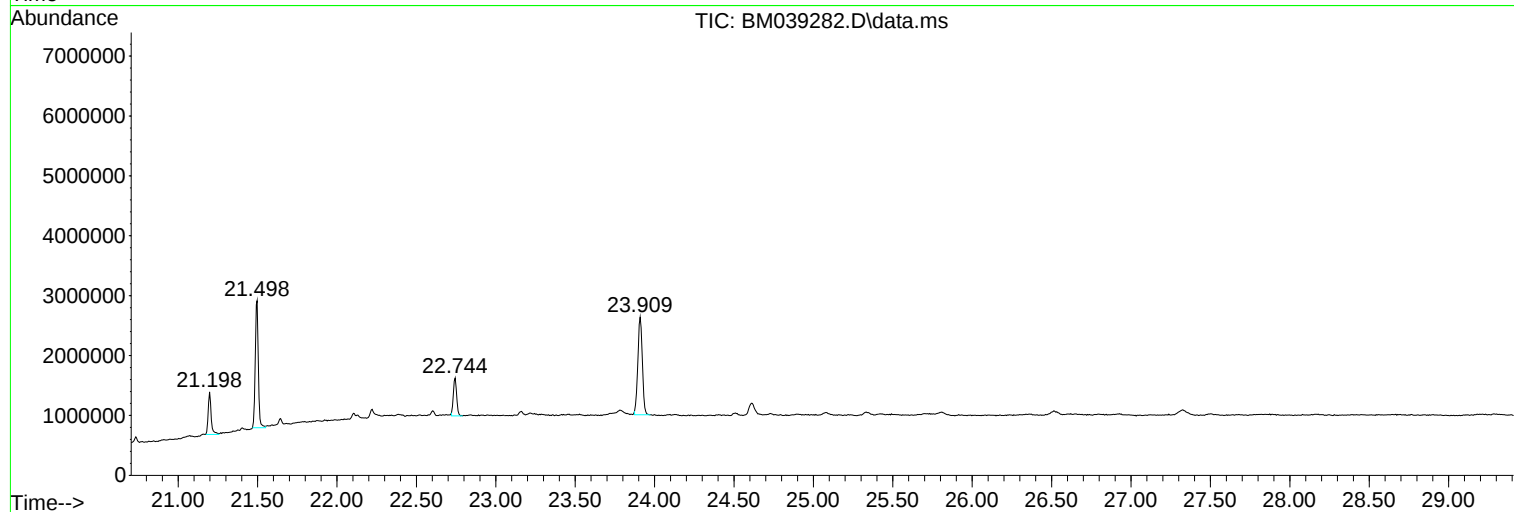
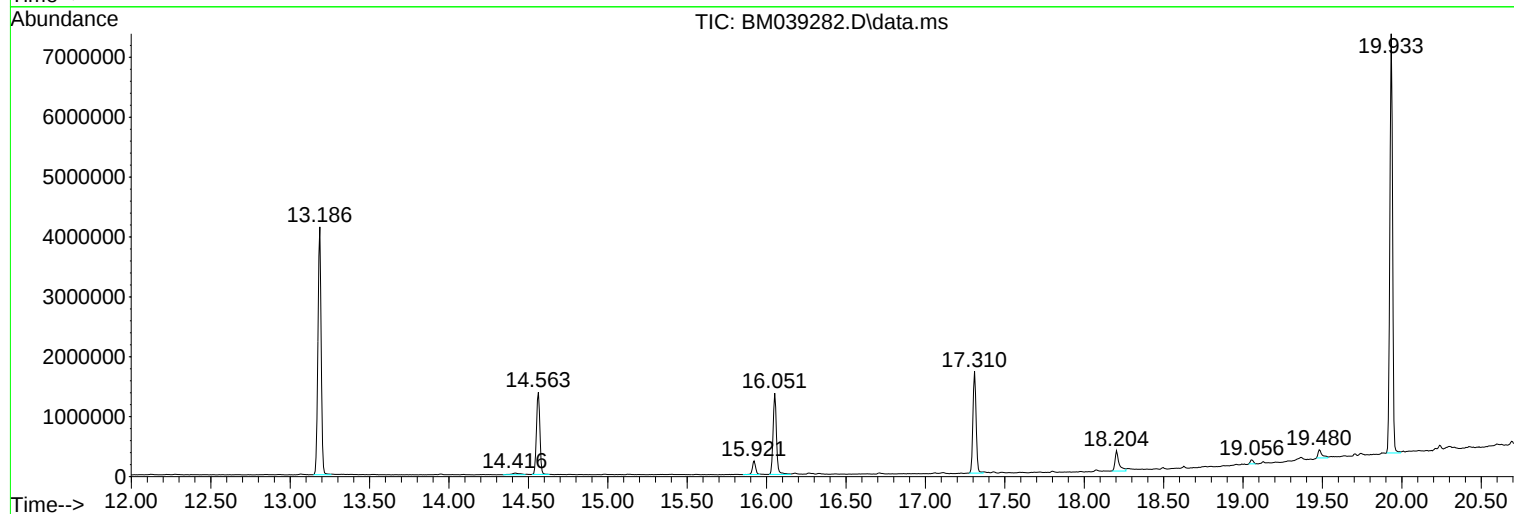
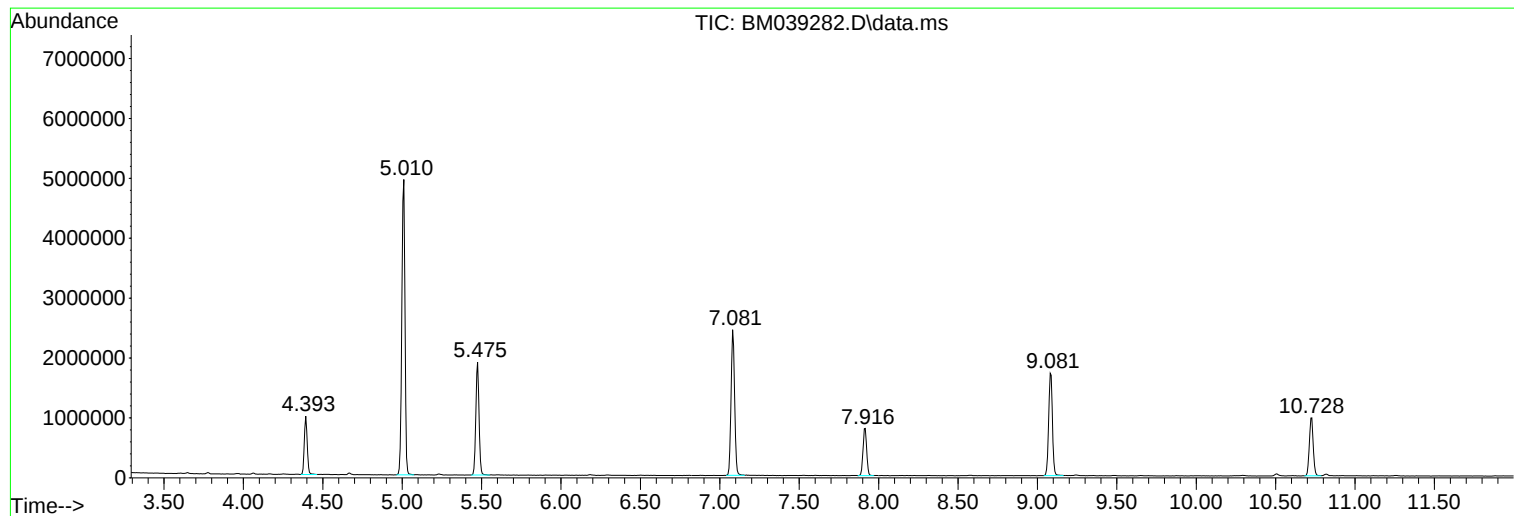
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.393	183	188	200	rVB	974176	1225586	14.82%	2.456%
2	5.010	285	293	304	rBV	4932433	6804845	82.27%	13.637%
3	5.475	365	372	385	rBV	1884355	2668165	32.26%	5.347%
4	7.081	638	645	658	rBV	2431641	3685127	44.56%	7.385%
5	7.916	779	787	796	rBV	786496	1256784	15.20%	2.519%
6	9.081	978	985	999	rBV	1711031	2819412	34.09%	5.650%
7	10.728	1257	1265	1275	rBV	967518	1658546	20.05%	3.324%
8	13.186	1676	1683	1695	rBV	4137529	5887904	71.19%	11.799%
9	14.416	1879	1892	1903	rBV6	27517	104402	1.26%	0.209%
10	14.563	1910	1917	1929	rBV	1373954	2021375	24.44%	4.051%
11	15.921	2136	2148	2154	rBV	228121	328525	3.97%	0.658%
12	16.051	2164	2170	2187	rBV	1356296	1986244	24.01%	3.980%
13	17.310	2378	2384	2393	rBV	1698628	2340948	28.30%	4.691%
14	18.204	2531	2536	2546	rBV	338008	599944	7.25%	1.202%
15	19.056	2678	2681	2685	rVB3	65993	86336	1.04%	0.173%
16	19.480	2750	2753	2762	rBV	134978	240102	2.90%	0.481%
17	19.933	2825	2830	2840	rBV	7001508	8270937	100.00%	16.575%
18	21.198	3041	3045	3055	rBV	709270	915253	11.07%	1.834%
19	21.498	3091	3096	3105	rBV	2121740	2874240	34.75%	5.760%
20	22.744	3304	3308	3316	rVB	632433	901312	10.90%	1.806%
21	23.909	3500	3506	3517	rVB2	1629872	3225198	38.99%	6.463%

Sum of corrected areas: 49901185

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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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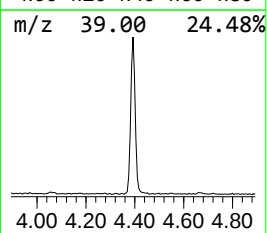
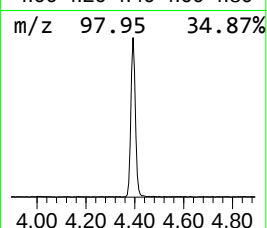
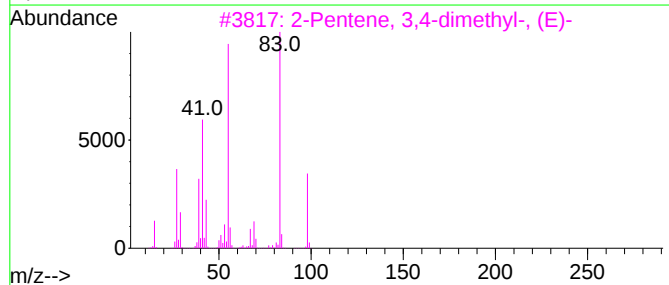
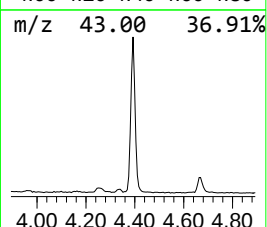
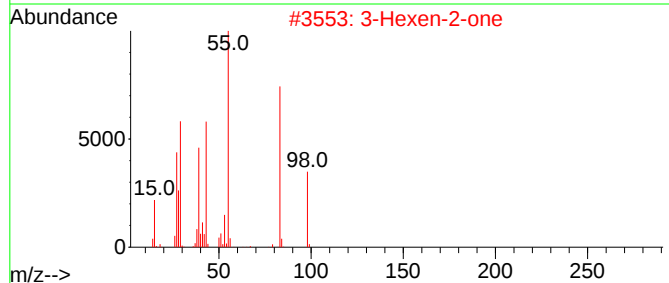
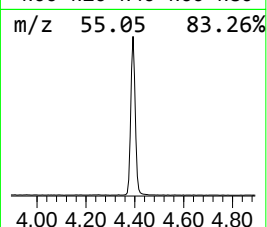
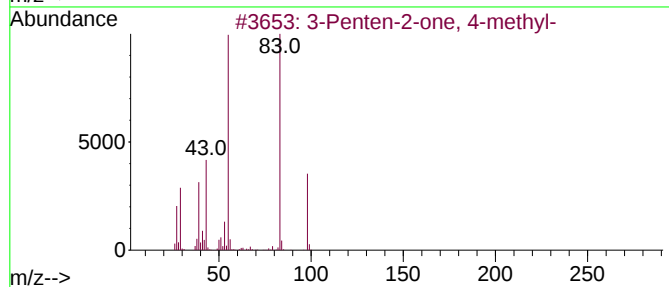
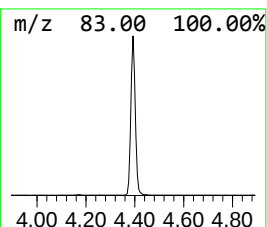
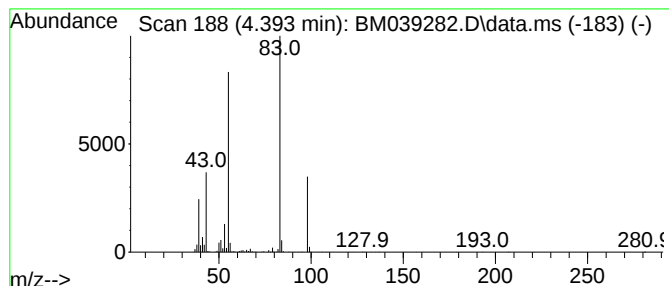
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.393	19.50 ng	1225590	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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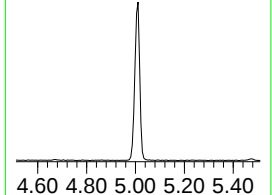
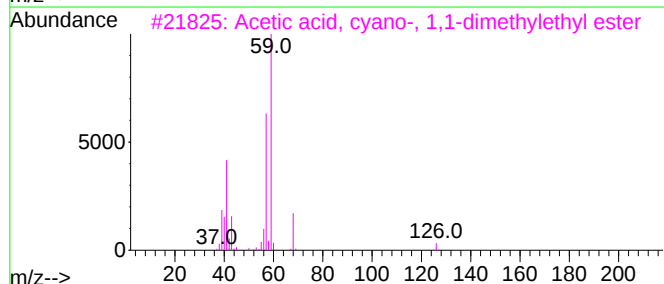
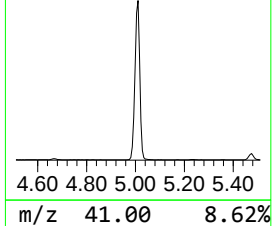
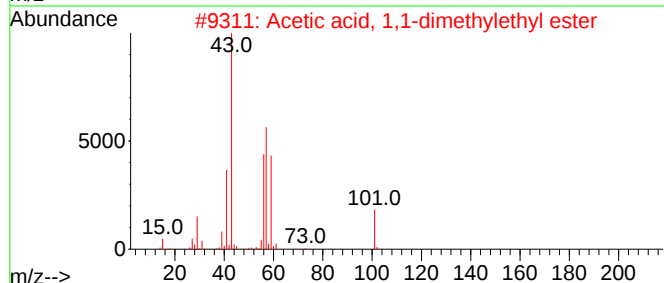
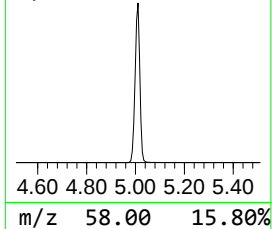
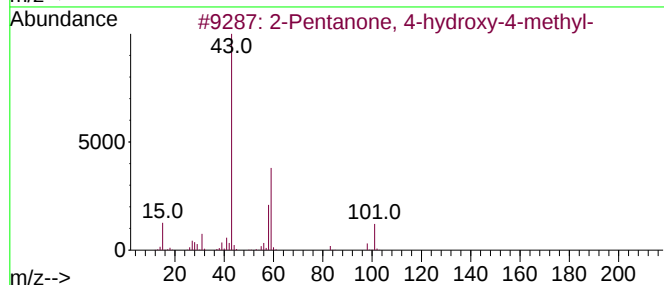
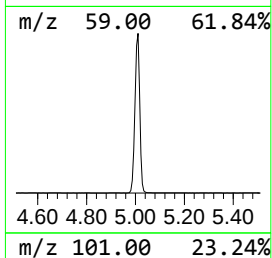
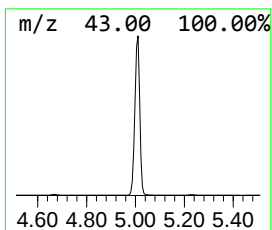
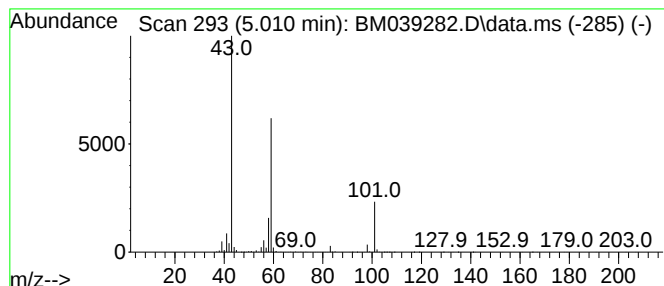
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.010	108.29 ng	6804850	1,4-Dichlorobenzene-d4	7.916

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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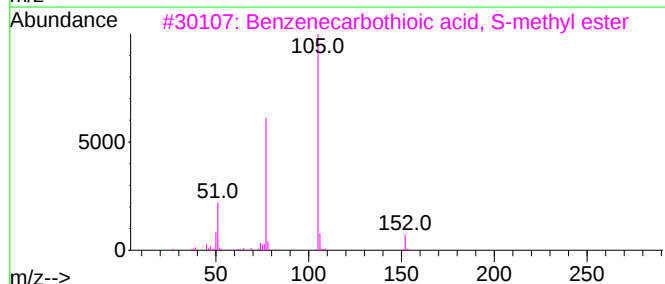
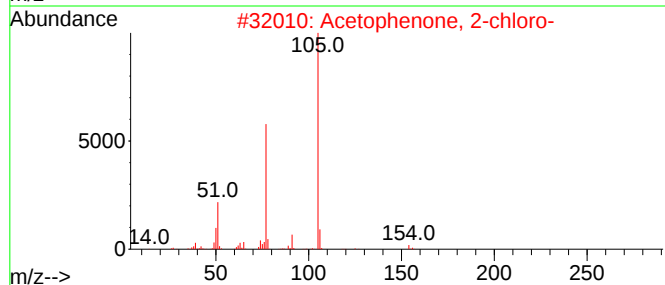
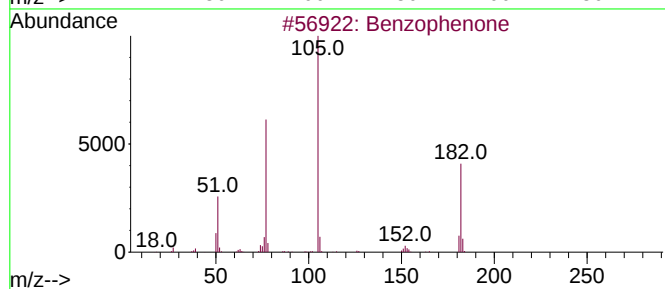
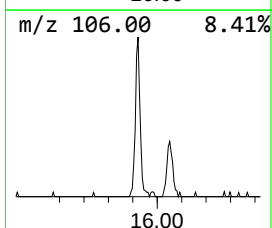
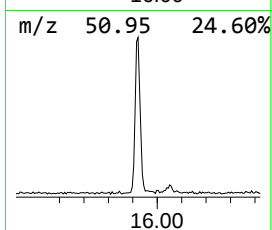
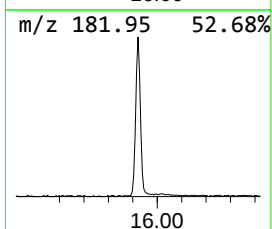
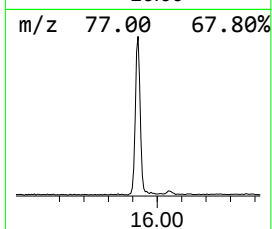
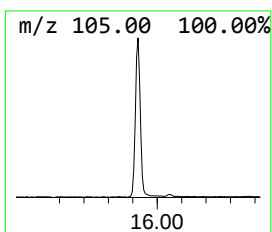
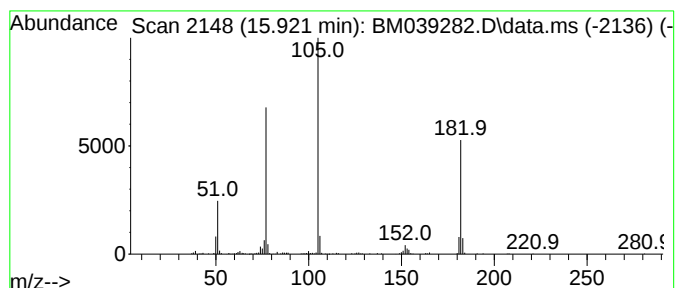
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Peak Number 3 Benzophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.921	3.25 ng	328525	Acenaphthene-d10	14.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	49
4			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
5			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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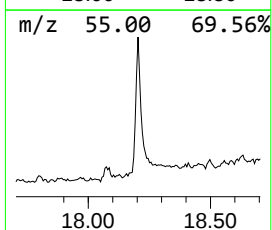
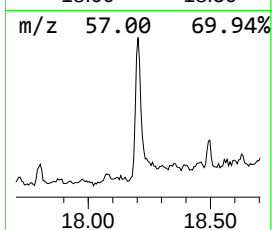
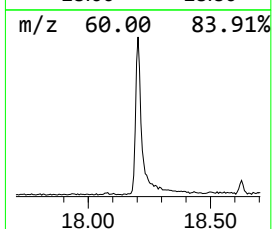
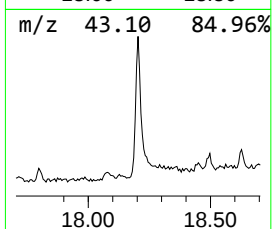
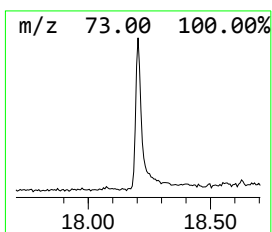
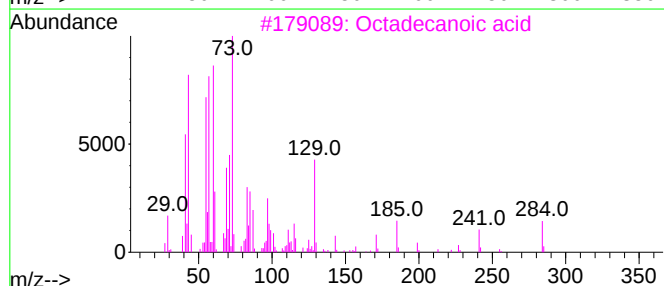
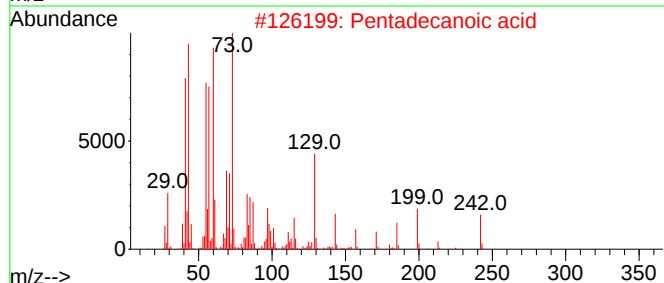
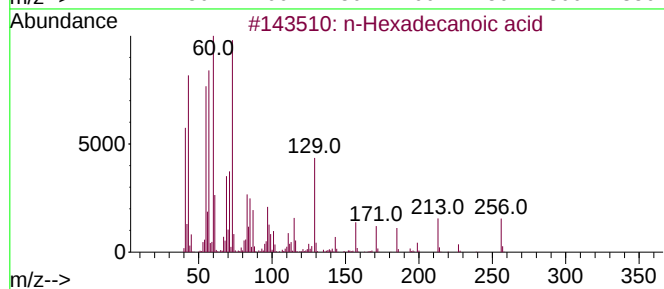
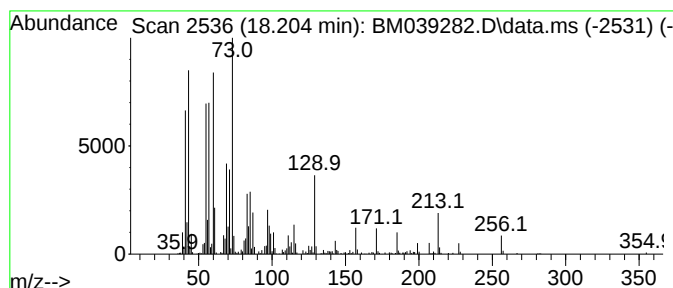
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.204	5.13 ng	599944	Phenanthrene-d10	17.310

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3		Octadecanoic acid	284	C18H36O2	000057-11-4	91
4		Tridecanoic acid	214	C13H26O2	000638-53-9	87
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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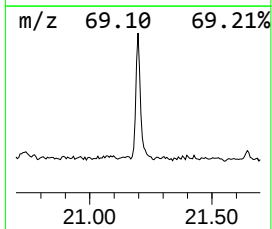
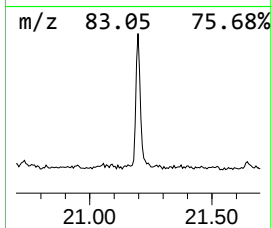
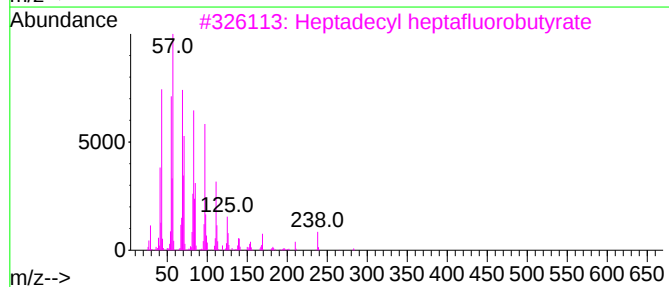
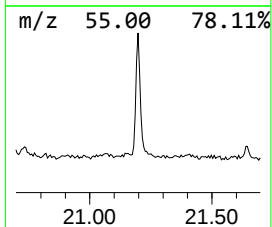
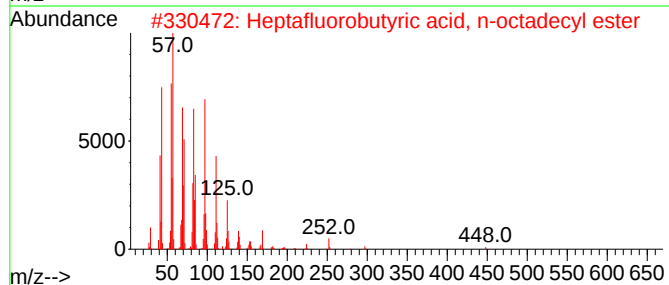
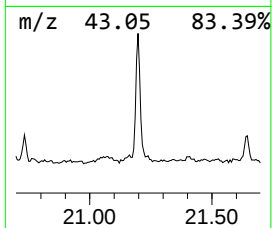
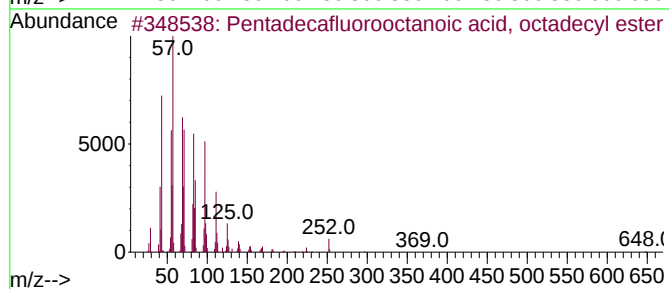
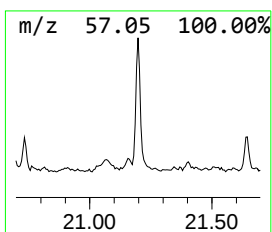
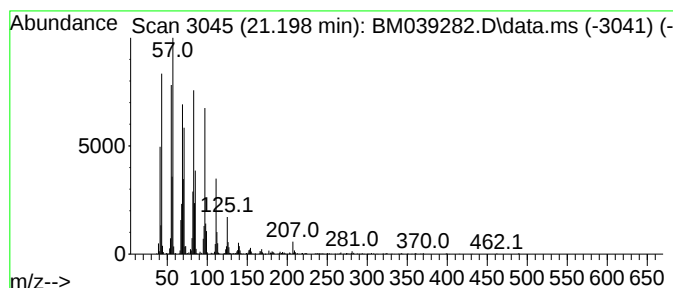
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Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.198	6.37 ng	915253	Chrysene-d12	21.497

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	94
3			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4			1-Hexacosene	364	C26H52	018835-33-1	93
5			Nonacos-1-ene	406	C29H58	018835-35-3	93



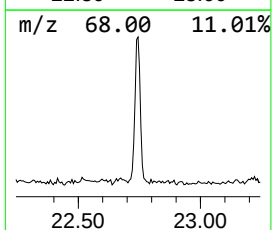
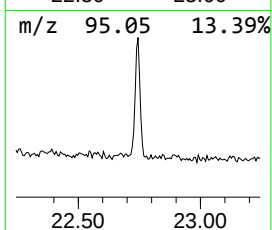
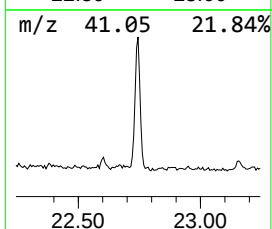
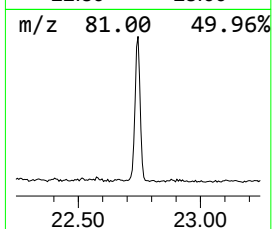
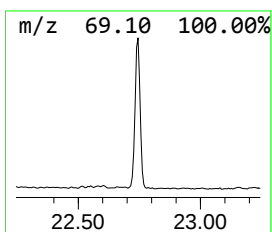
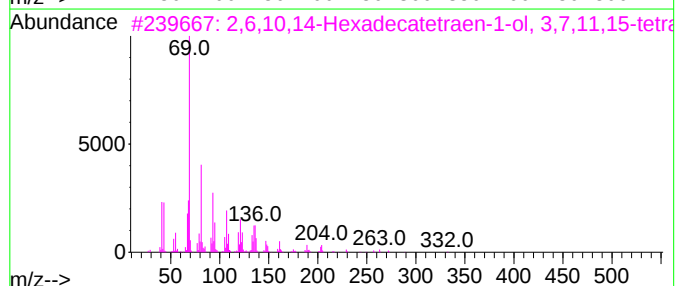
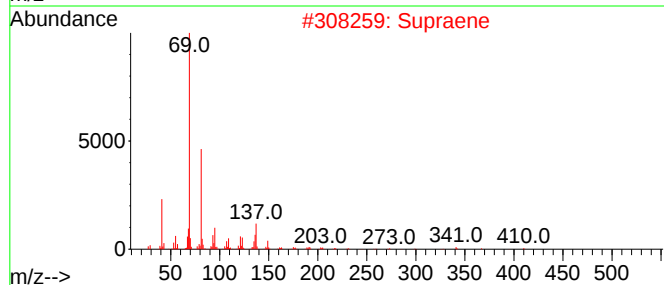
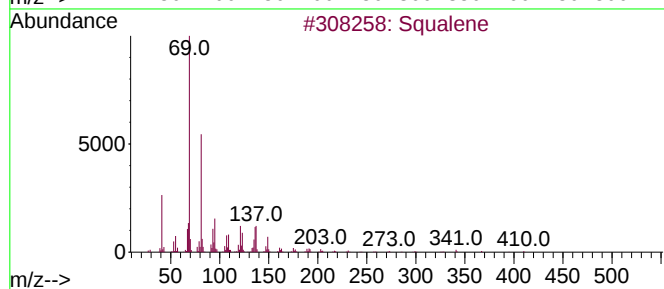
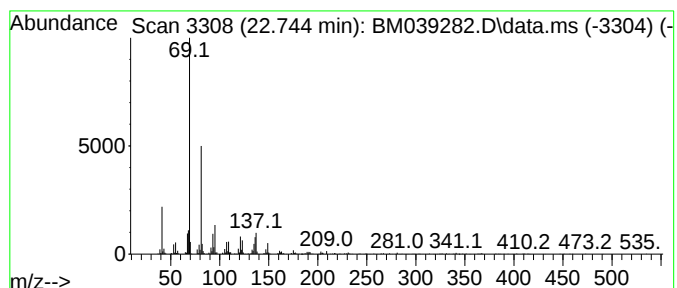
Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039282.D
Acq On : 03 Apr 2023 16:58
Operator : CG/JU
Sample : 02154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.744	5.59 ng	901312	Perylene-d12	23.909	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Squalene	410	C30H50	000111-02-4	94
2	Supraene	410	C30H50	007683-64-9	91
3	2,6,10,14-Hexadecatetraen-1-ol, ...	332	C22H36O2	061691-98-3	72
4	4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
5	Farnesol isomer a	222	C15H26O	1000108-92-4	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040323\
Data File : BM039282.D
Acq On : 03 Apr 2023 16:58
Operator : CG/JU
Sample : 02154-01
Misc :
ALS Vial : 11 Sample Multiplier: 1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM032923.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
3-Penten-2-one,...	4.393	19.5	ng	1225590	1	7.916	1256780	20.0
2-Pentanone, 4-...	5.010	108.3	ng	6804850	1	7.916	1256780	20.0
Benzophenone	15.921	3.3	ng	328525	3	14.563	2021380	20.0
n-Hexadecanoic ...	18.204	5.1	ng	599944	4	17.310	2340950	20.0
Pentadecafluoro...	21.198	6.4	ng	915253	5	21.497	2874240	20.0
Squalene	22.744	5.6	ng	901312	6	23.909	3225200	20.0