

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF031523\
 Data File : BF132804.D
 Acq On : 15 Mar 2023 15:41
 Operator : CG\JU
 Sample : 01908-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HILLBOR-DRUMS-0314

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_F\Methods\8270-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.204	440	445	463	rVB	1685134	2343258	43.94%	6.027%
2	5.604	508	513	527	rBV	4240314	4685949	87.88%	12.052%
3	6.598	677	682	685	rBV	4234025	4692275	88.00%	12.068%
4	6.963	741	744	748	rBV	1510925	1207571	22.65%	3.106%
5	7.533	836	841	844	rBV	3161326	3157617	59.22%	8.121%
6	8.245	959	962	966	rBV	1745280	1494154	28.02%	3.843%
7	9.322	1141	1145	1148	rBV	5743870	5332384	100.00%	13.715%
8	10.004	1258	1261	1265	rBV	2049780	1891912	35.48%	4.866%
9	10.721	1379	1383	1386	rVB	434369	376183	7.05%	0.968%
10	10.804	1392	1397	1400	rBV	3595578	3504154	65.71%	9.013%
11	11.498	1512	1515	1519	rBV	2118786	1952920	36.62%	5.023%
12	12.015	1597	1603	1617	rBV2	497228	687842	12.90%	1.769%
13	12.257	1641	1644	1649	rVB	73767	68404	1.28%	0.176%
14	12.721	1718	1723	1729	rBV8	24948	54682	1.03%	0.141%
15	12.798	1732	1736	1746	rBV2	107304	168709	3.16%	0.434%
16	13.092	1781	1786	1789	rVB	4760182	4787451	89.78%	12.313%
17	13.980	1933	1937	1954	rBV3	155782	376568	7.06%	0.969%
18	14.151	1963	1966	1978	rVB	1234212	1255492	23.54%	3.229%
19	15.203	2138	2145	2147	rBV7	48227	101743	1.91%	0.262%
20	15.686	2222	2227	2234	rBV	550474	741576	13.91%	1.907%

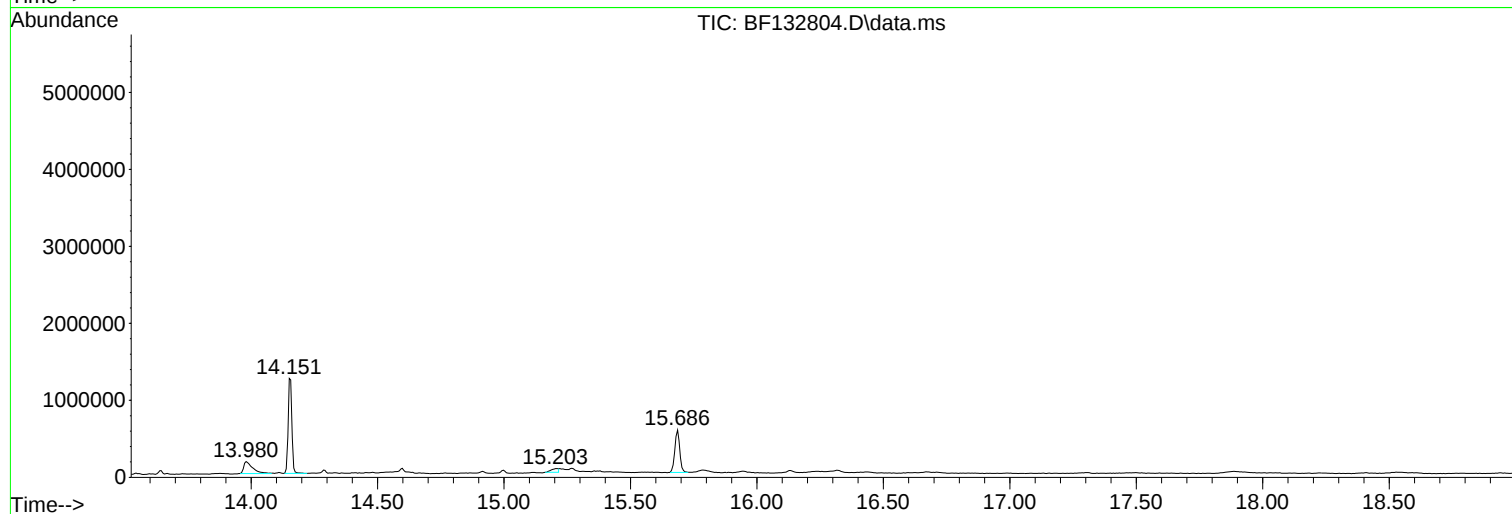
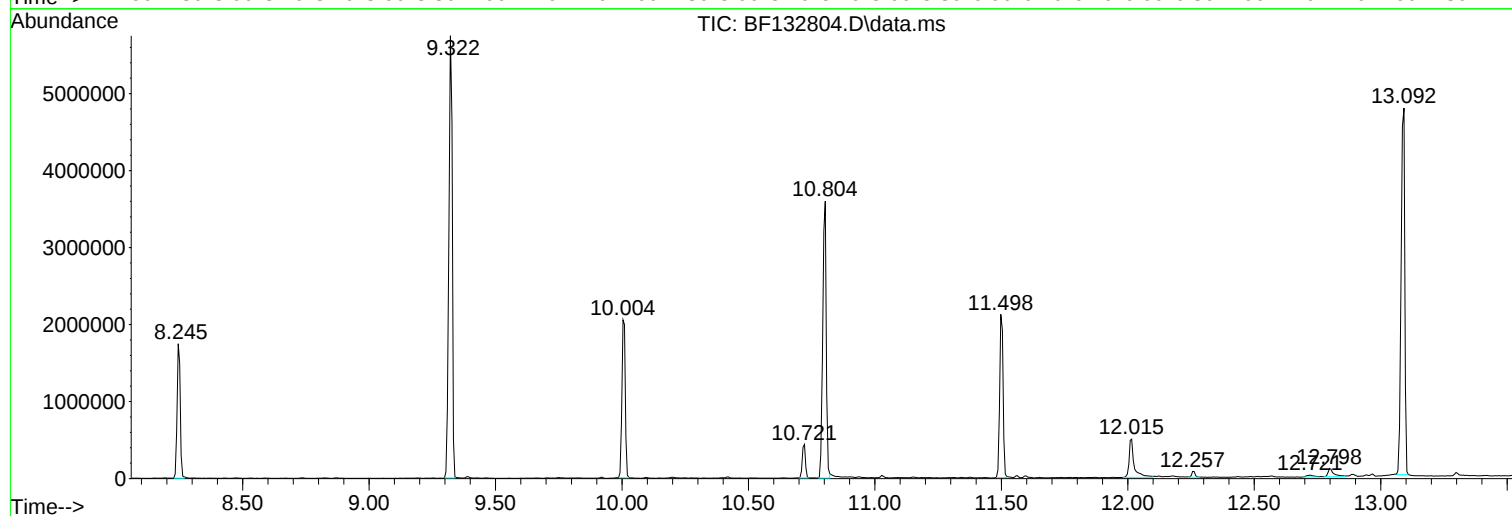
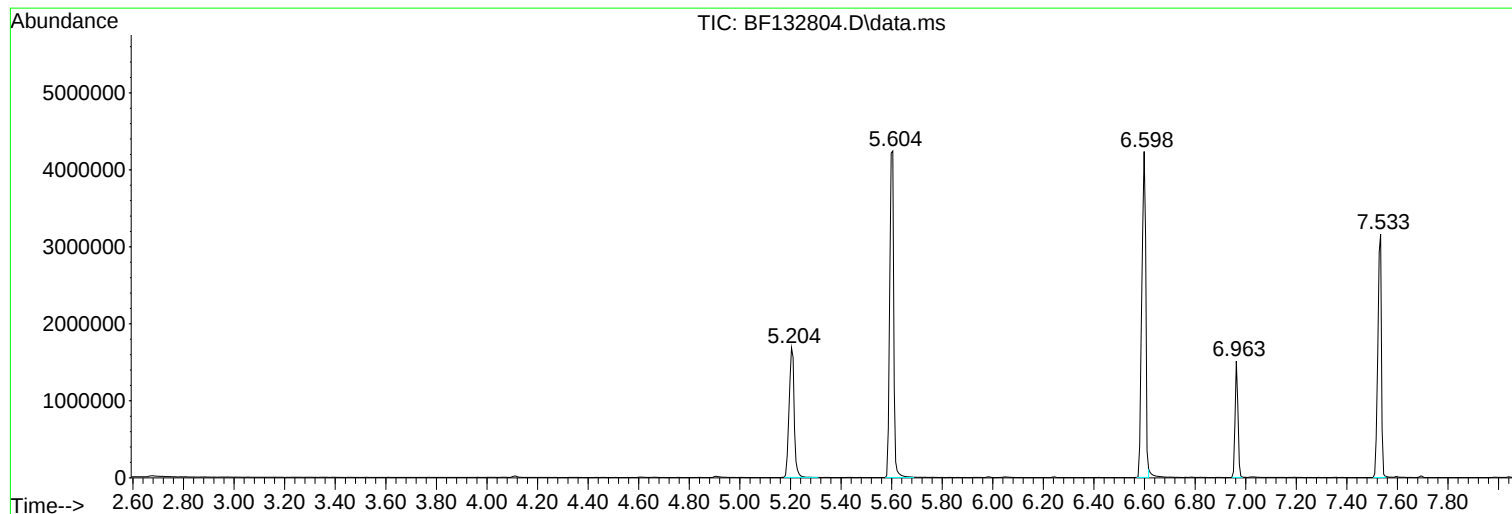
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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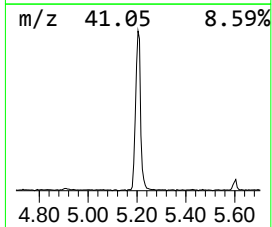
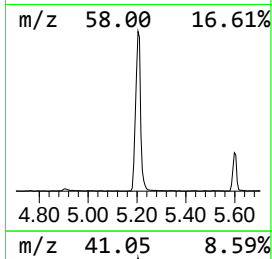
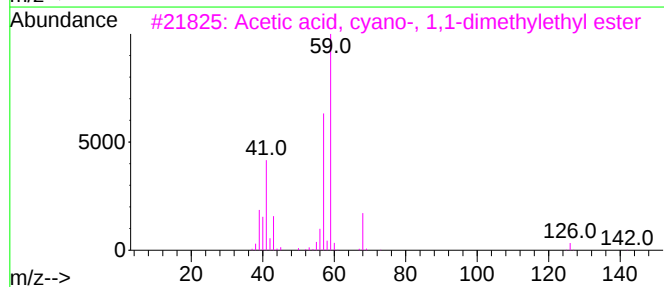
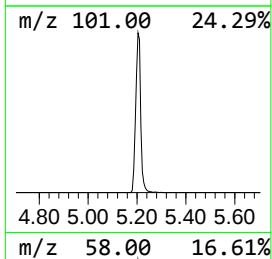
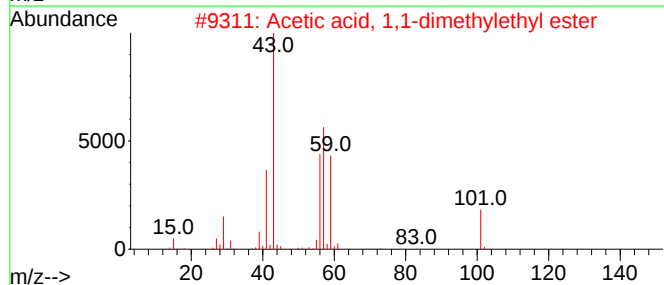
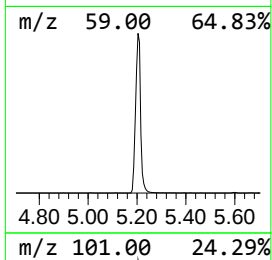
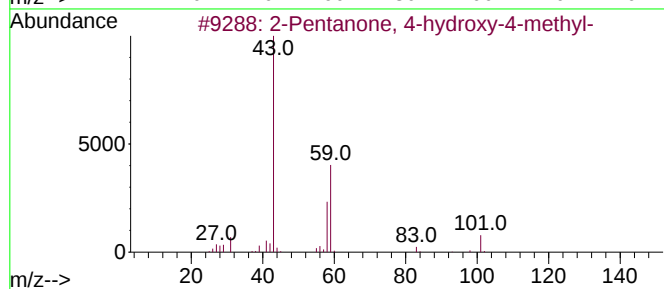
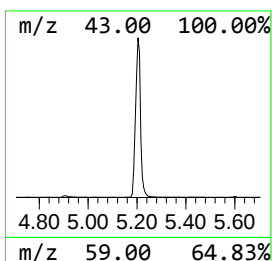
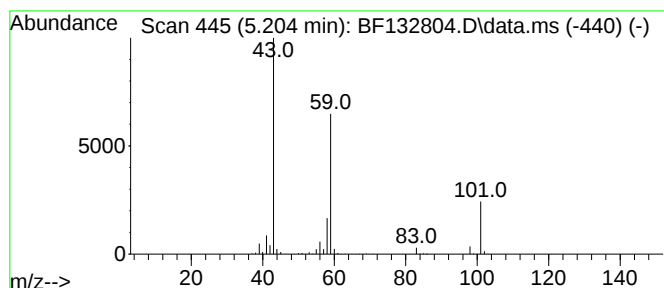
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.204	38.81 ng	2343260	1,4-Dichlorobenzene-d4	6.963

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
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	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	5-Hexen-2-one	98	C6H10O	000109-49-9	9		



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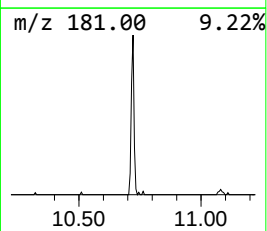
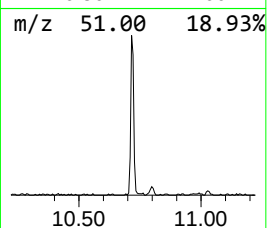
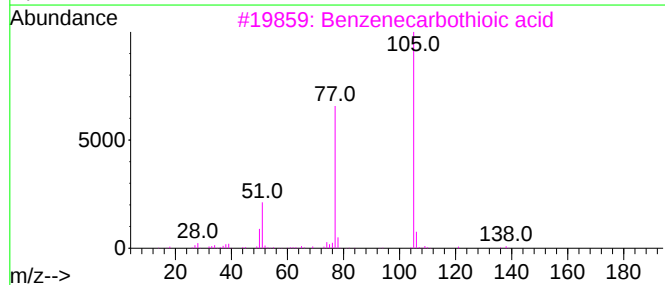
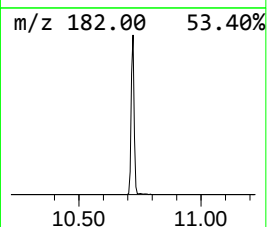
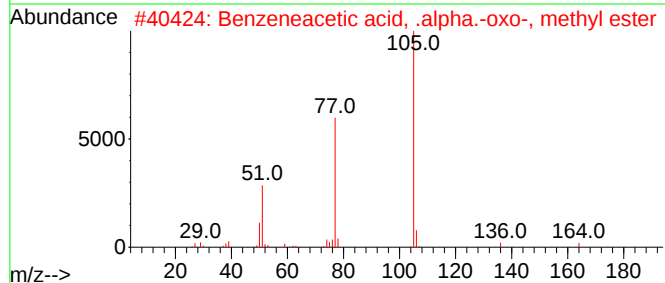
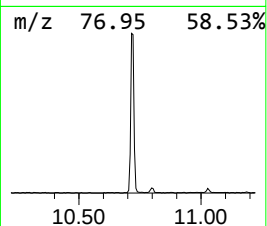
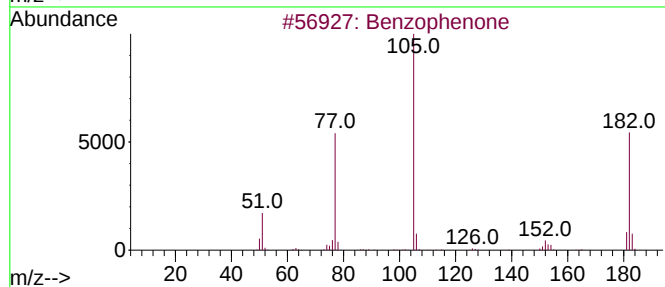
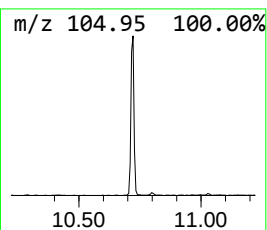
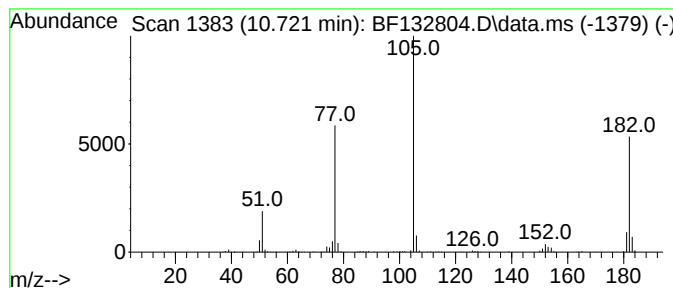
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.721	3.98 ng	376183	Acenaphthene-d10	10.004

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	43
3			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	43
4			Methyl 2-benzoyl-4-cyanobutanoate	231	C13H13NO3	1010486-83-8	43
5			Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	43



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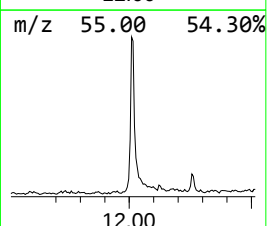
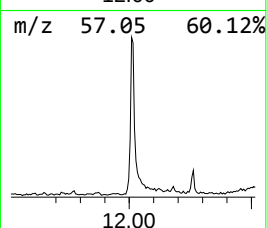
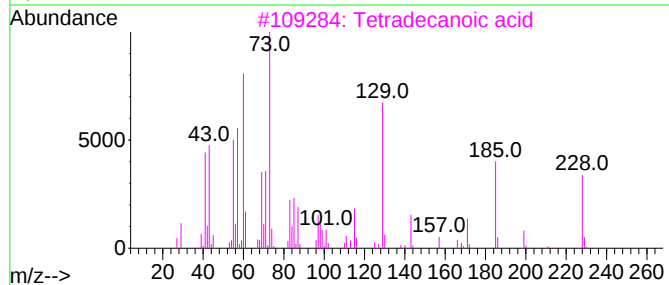
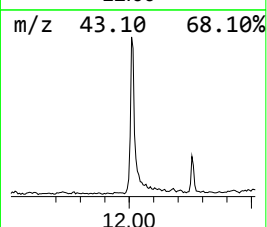
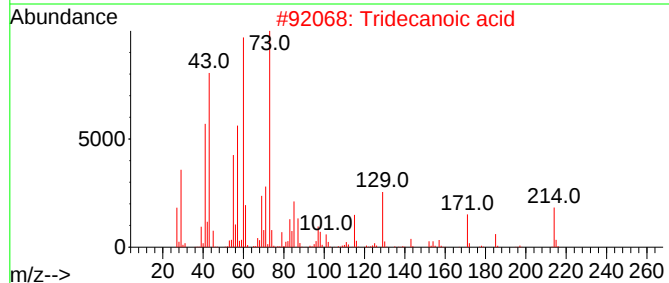
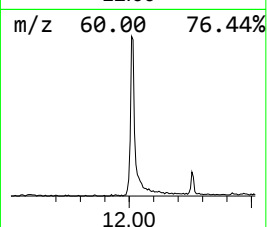
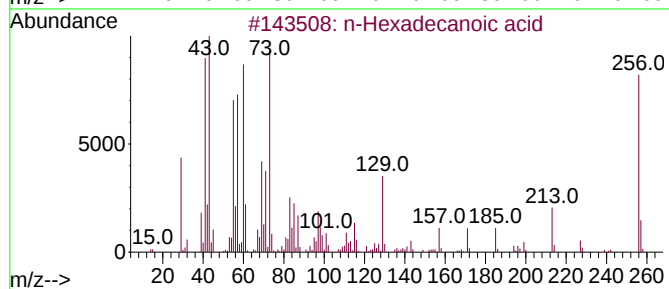
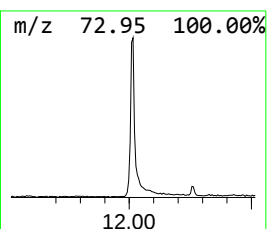
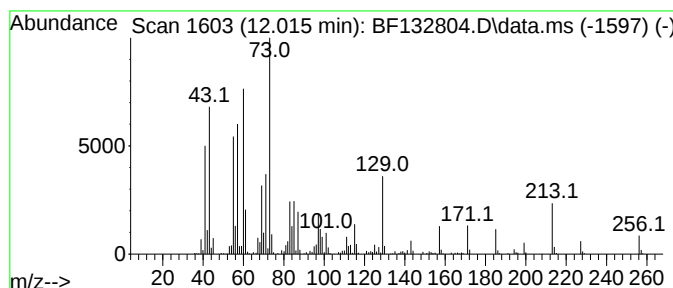
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.015	7.04 ng	687842	Phenanthrene-d10	11.498

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Dodecanoic acid	200	C12H24O2	000143-07-7	53



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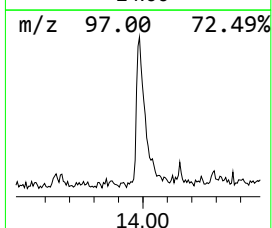
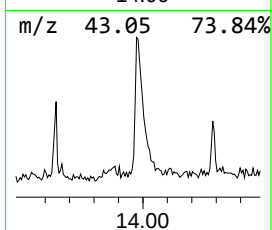
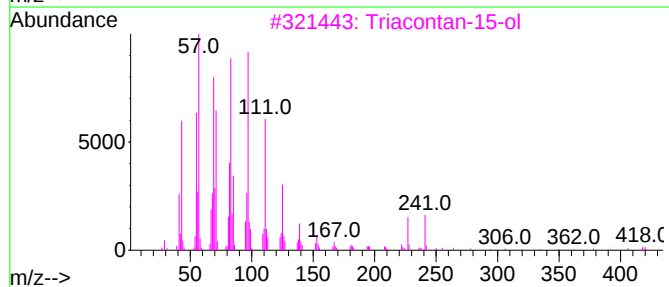
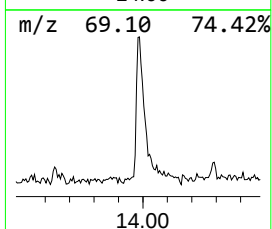
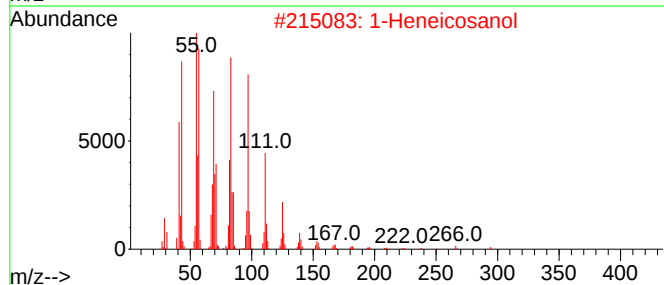
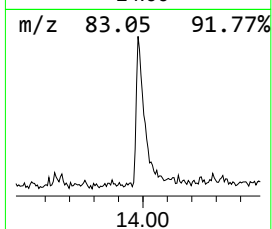
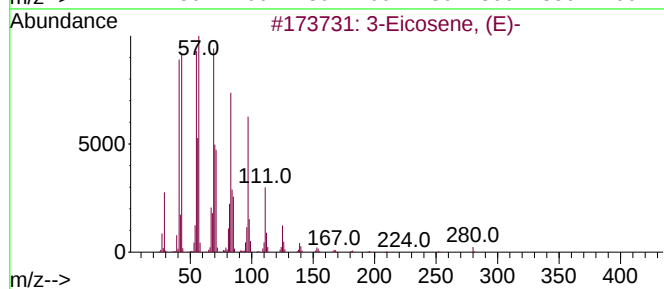
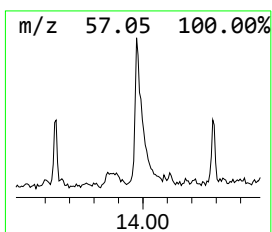
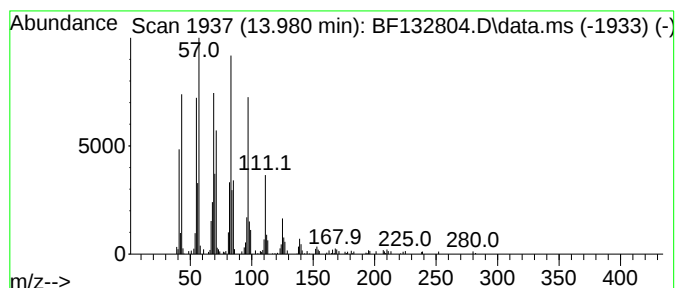
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Peak Number 4 3-Eicosene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.980	6.00 ng	376568	Chrysene-d12	14.156

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2			1-Heneicosanol	312	C21H44O	015594-90-8	93
3			Triacontan-15-ol	438	C30H62O	031849-26-0	91
4			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
5			2-Chloropropionic acid, octadec...	360	C21H41ClO2	088104-31-8	91



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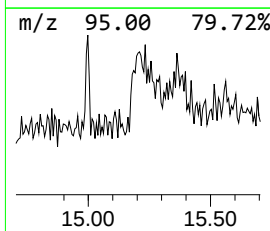
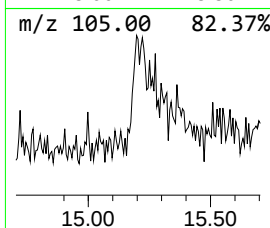
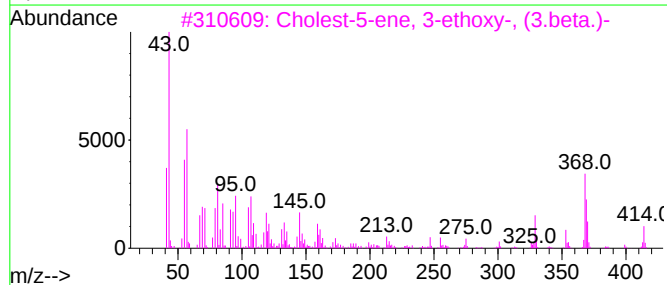
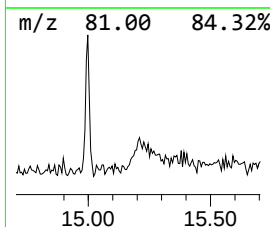
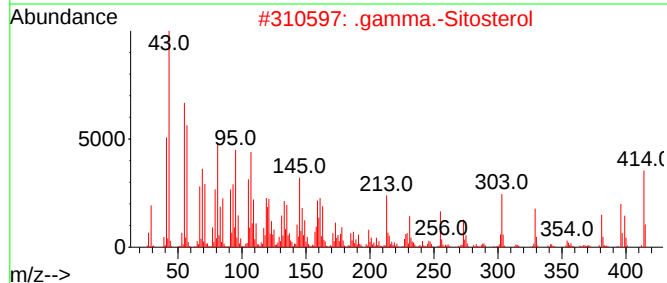
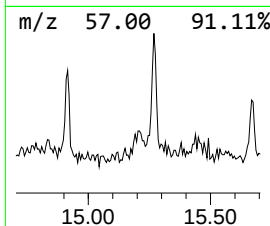
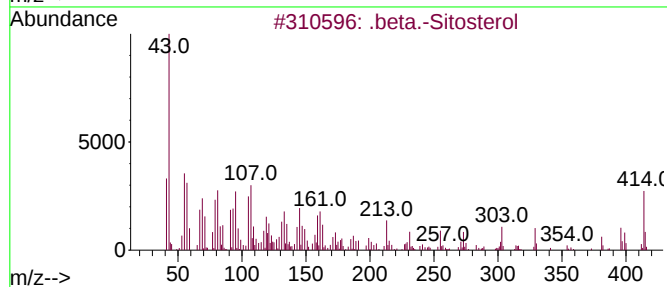
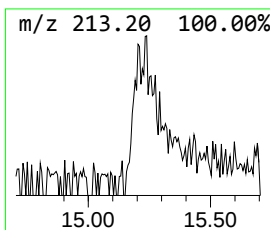
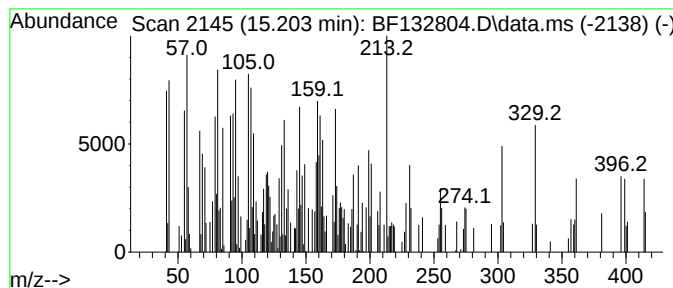
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 .beta.-Sitosterol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.204	2.74 ng	101743	Perylene-d12	15.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.beta.-Sitosterol	414	C29H50O	000083-46-5	95
2			.gamma.-Sitosterol	414	C29H50O	000083-47-6	64
3			Cholest-5-ene, 3-ethoxy-, (3.beta...	414	C29H50O	000986-19-6	55
4			Carbamothioic acid, (1,7,7-trime...	303	C18H25NOS	1000337-85-0	35
5			2,4-Hexadienamide, N-(4-methylph...	201	C13H15NO	1000362-68-5	30



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.204	38.8	ng	2343260	1	6.963	1207570	20.0
Benzophenone	10.721	4.0	ng	376183	3	10.004	1891910	20.0
n-Hexadecanoic ...	12.015	7.0	ng	687842	4	11.498	1952920	20.0
3-Eicosene, (E)-	13.980	6.0	ng	376568	5	14.156	1255490	20.0
.beta.-Sitosterol	15.204	2.7	ng	101743	6	15.686	741576	20.0