

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011023\
 Data File : BF131992.D
 Acq On : 10 Jan 2023 12:06
 Operator : CG\JU
 Sample : 01064-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S4-02

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-BF010923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131992.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	487	493	504	rVB	598220	851941	33.05%	5.069%
2	5.404	559	564	567	rBV	2116471	1940936	75.30%	11.549%
3	6.428	733	738	741	rBV	1929195	2010167	77.98%	11.961%
4	6.787	795	799	802	rBV	473194	425048	16.49%	2.529%
5	7.357	891	896	899	rBV	1436974	1326044	51.44%	7.890%
6	8.075	1013	1018	1021	rBV	669647	549039	21.30%	3.267%
7	9.157	1197	1202	1205	rBV	2690530	2417637	93.79%	14.386%
8	9.833	1313	1317	1320	rBV	812952	664142	25.77%	3.952%
9	10.551	1435	1439	1443	rVB	109470	91048	3.53%	0.542%
10	10.633	1448	1453	1456	rBV	1834687	1772871	68.78%	10.549%
11	11.327	1567	1571	1574	rBV	917588	728180	28.25%	4.333%
12	11.857	1656	1661	1664	rBV	56889	64617	2.51%	0.384%
13	12.010	1681	1687	1691	rBV2	23568	31929	1.24%	0.190%
14	12.051	1691	1694	1700	rVB4	19732	29620	1.15%	0.176%
15	12.921	1837	1842	1845	rBV	3031282	2577658	100.00%	15.338%
16	13.616	1955	1960	1969	rBV4	17694	35616	1.38%	0.212%
17	13.827	1992	1996	2006	rBV	122069	218681	8.48%	1.301%
18	13.974	2017	2021	2025	rBV	530693	481280	18.67%	2.864%
19	14.210	2057	2061	2067	rVB4	21135	32243	1.25%	0.192%
20	15.445	2266	2271	2278	rVB	327208	426868	16.56%	2.540%
21	16.333	2416	2422	2429	rBV9	42480	130271	5.05%	0.775%

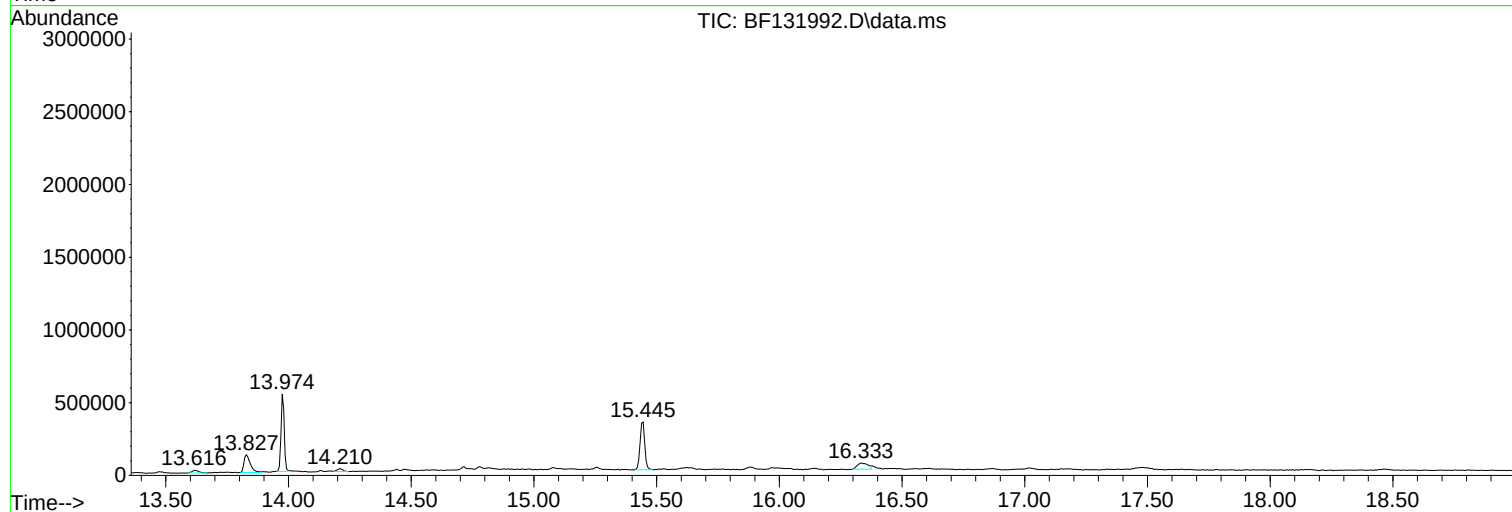
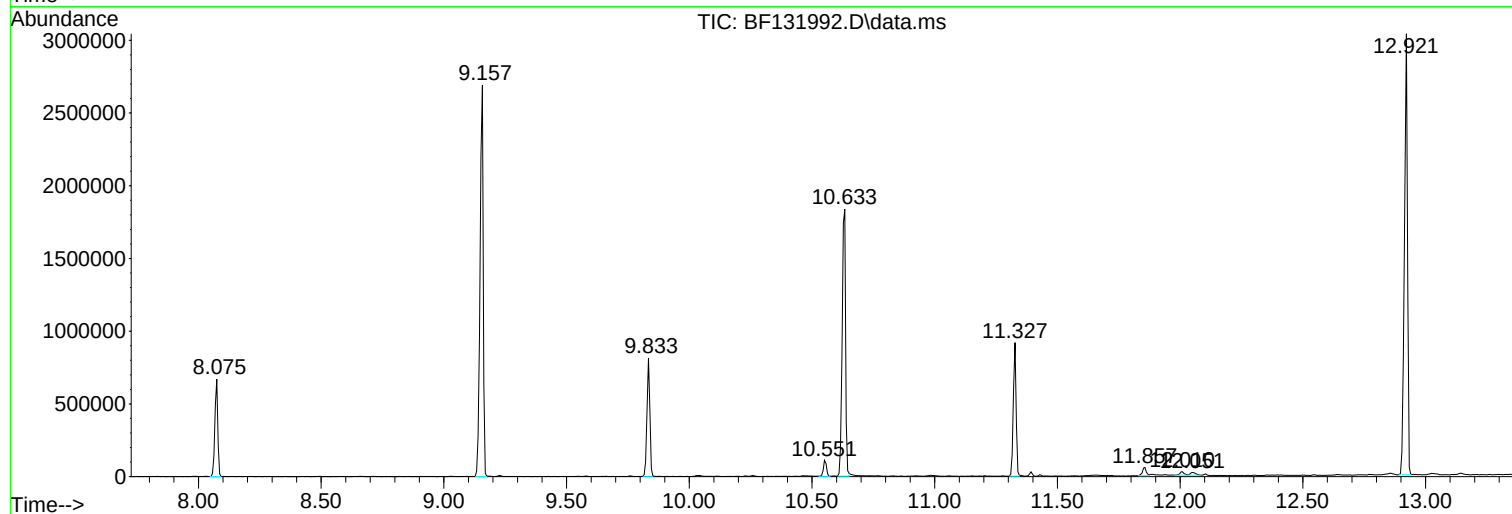
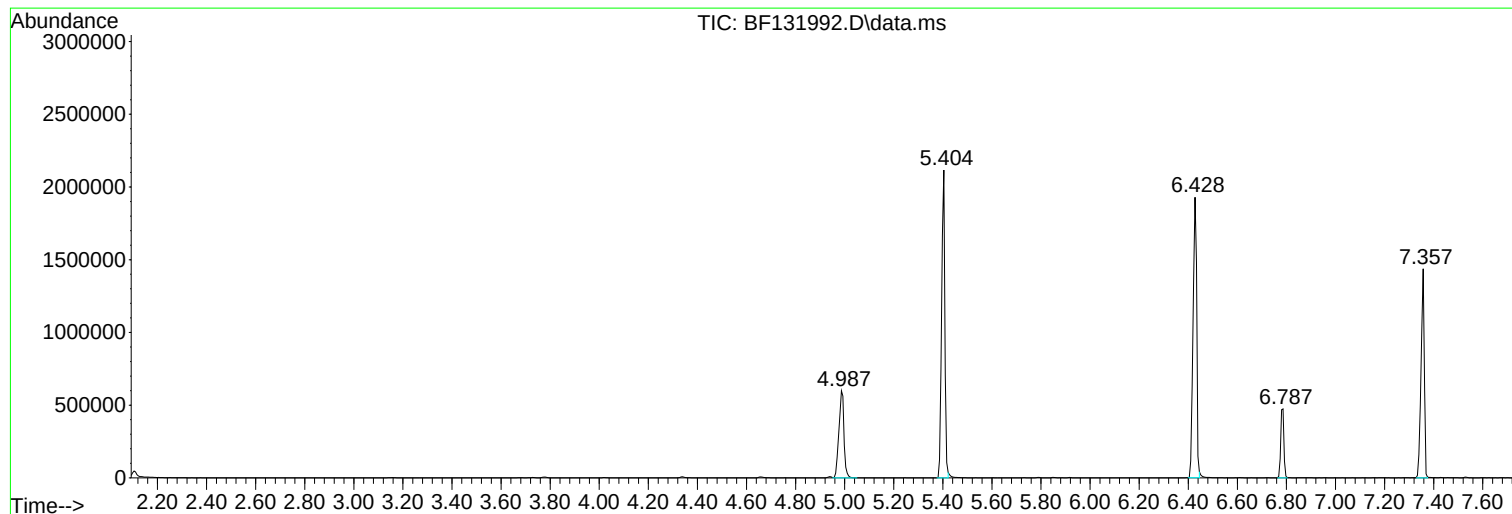
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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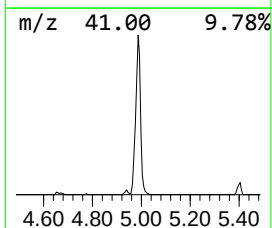
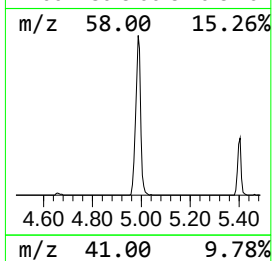
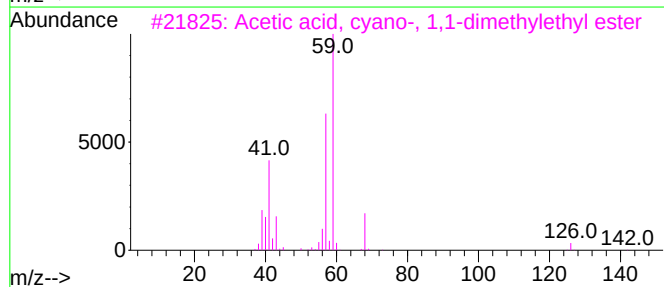
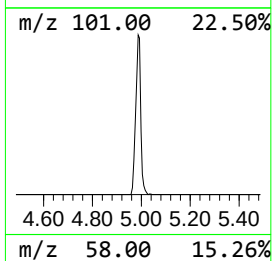
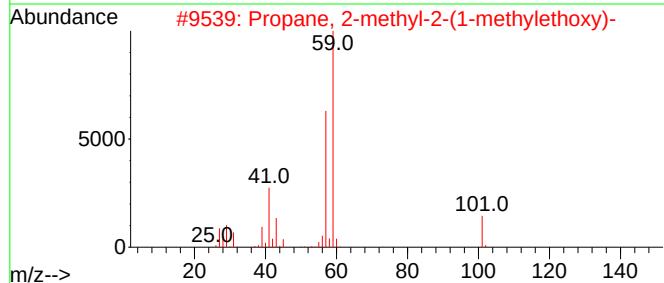
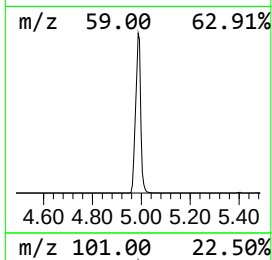
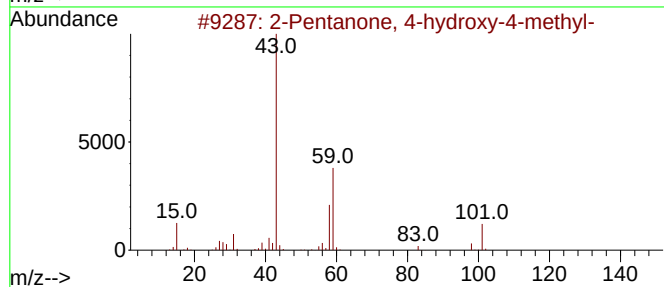
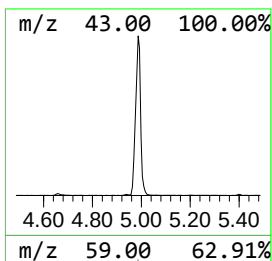
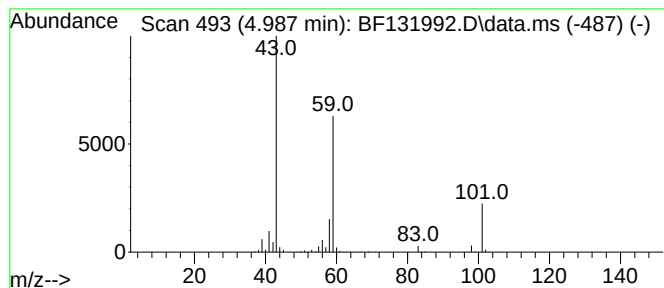
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	40.09 ng	851941	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53		
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	17		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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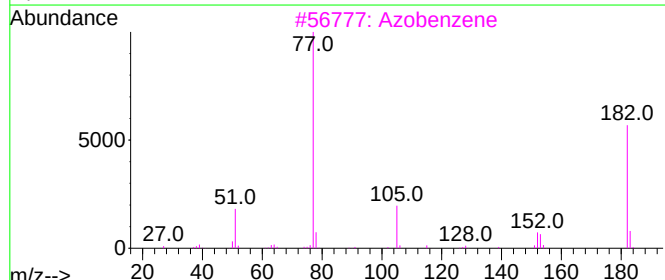
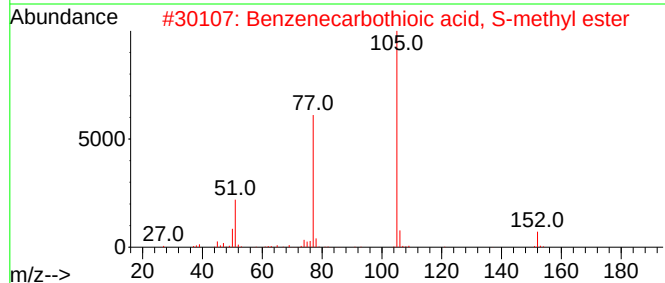
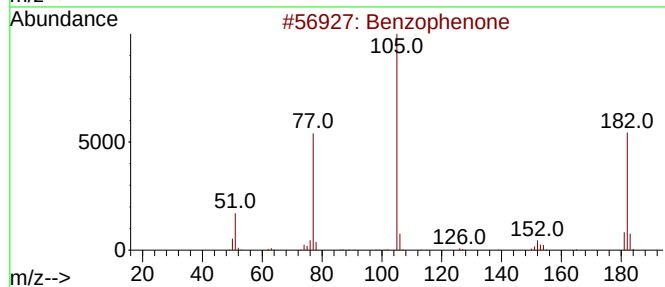
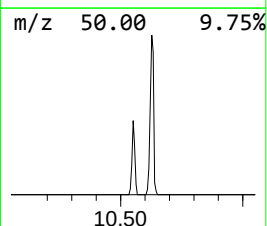
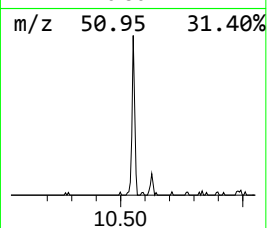
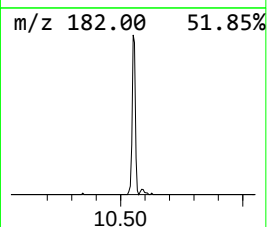
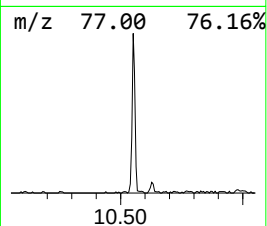
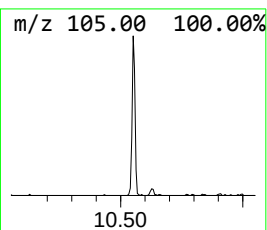
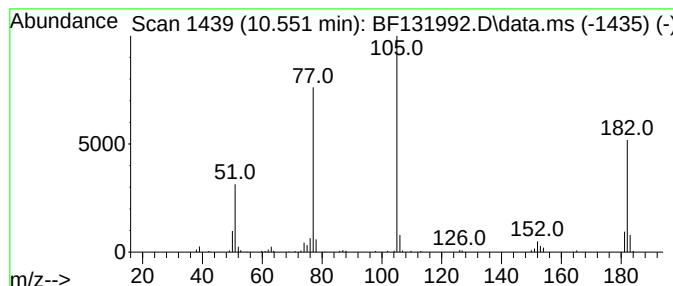
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.551	2.74 ng	91048	Acenaphthene-d10	9.833

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	70
3			Azobenzene	182	C12H10N2	000103-33-3	64
4			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	62
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	53



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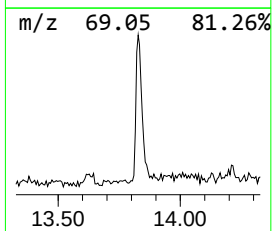
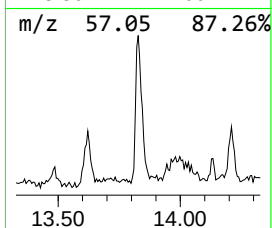
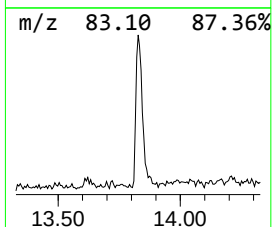
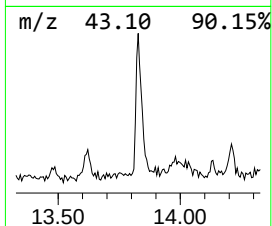
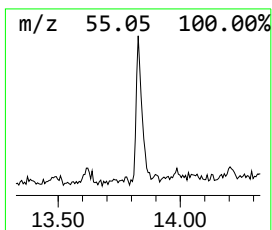
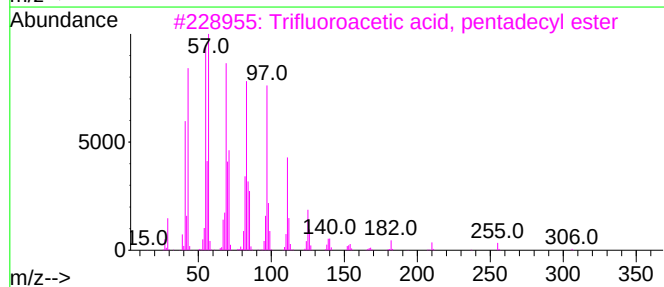
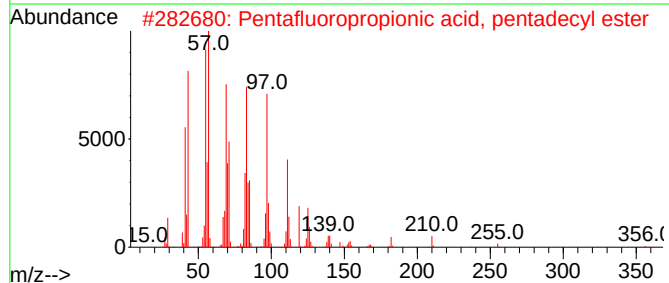
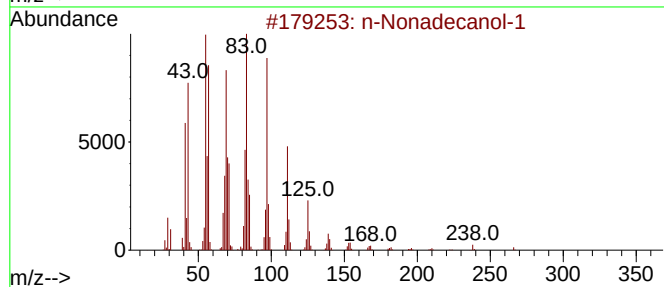
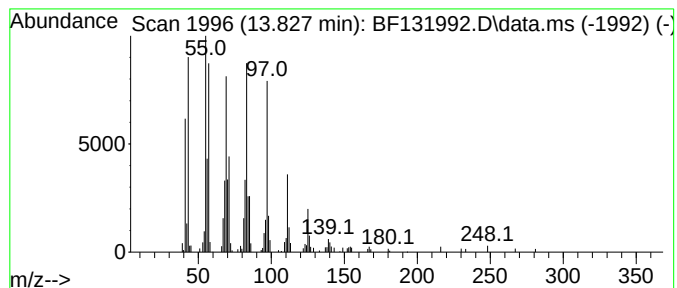
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Peak Number 3 n-Nonadecanol-1 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.827	9.09 ng	218681	Chrysene-d12	13.974

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Nonadecanol-1			284	C19H40O	001454-84-8	95
2	Pentafluoropropionic acid, penta...			374	C18H31F5O2	959092-08-1	95
3	Trifluoroacetic acid, pentadecyl...			324	C17H31F3O2	959010-23-2	95
4	1-Hexacosene			364	C26H52	018835-33-1	94
5	n-Tetracosanol-1			354	C24H50O	000506-51-4	94



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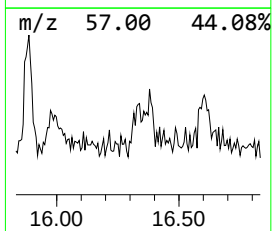
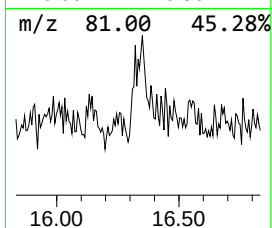
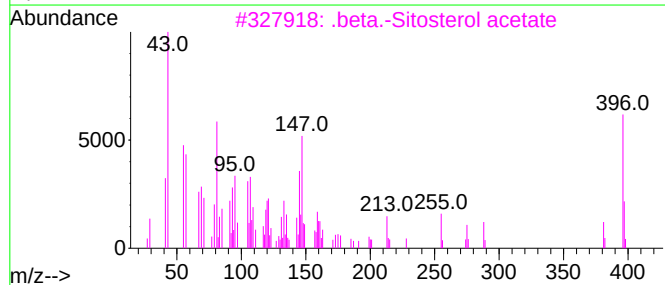
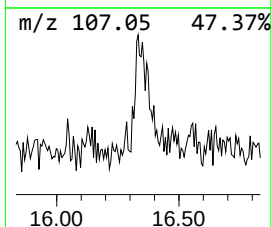
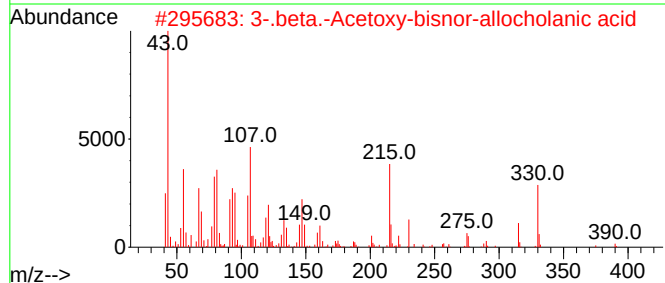
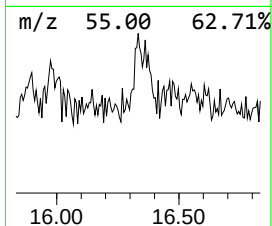
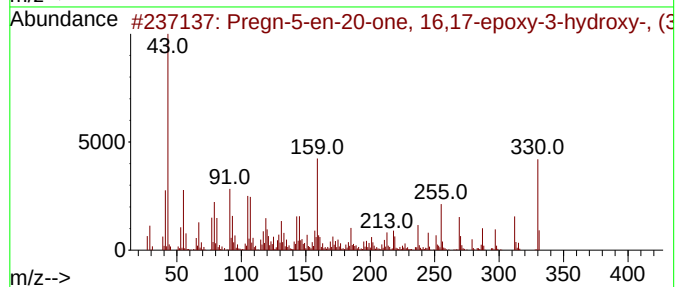
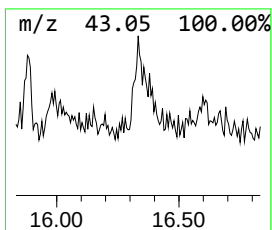
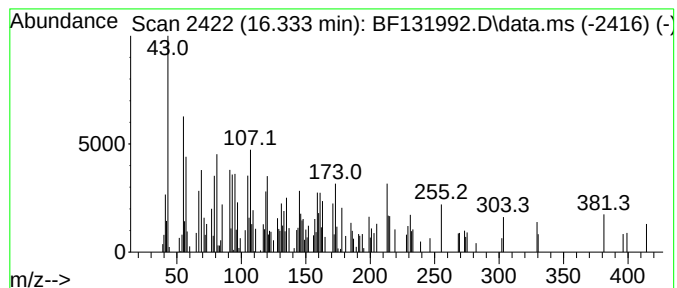
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Peak Number 4 unknown16.333 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.333	6.10 ng	130271	Perylene-d12	15.445

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pregn-5-en-20-one, 16,17-epoxy-3...	330	C21H30O3	000974-23-2	30
2			3-.beta.-Acetoxy-bisnor-allochol...	390	C24H38O4	1000226-91-3	22
3			.beta.-Sitosterol acetate	456	C31H52O2	000915-05-9	12
4			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	10
5			Stigmasta-3,5-diene	396	C29H48	004970-37-0	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.987	40.1	ng	851941	1	6.787	425048	20.0
Benzophenone	10.551	2.7	ng	91048	3	9.833	664142	20.0
n-Nonadecanol-1	13.827	9.1	ng	218681	5	13.974	481280	20.0
unknown16.333	16.333	6.1	ng	130271	6	15.445	426868	20.0