

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM080222\
 Data File : BM036051.D
 Acq On : 02 Aug 2022 14:32
 Operator : CG/JU
 Sample : N3927-11
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 RVE-84

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-BM080122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM036051.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.434	392	399	412	rBV	4493153	6278423	30.72%	7.127%
2	7.040	664	672	688	rBV	4146401	6323907	30.95%	7.178%
3	7.869	803	813	820	rBV	1081756	1663684	8.14%	1.888%
4	9.040	1004	1012	1024	rBV	2466021	4016814	19.66%	4.559%
5	10.675	1282	1290	1301	rBV	1393322	2311107	11.31%	2.623%
6	13.134	1700	1708	1722	rBV	6271046	8817527	43.15%	10.009%
7	14.504	1934	1941	1950	rBV	1924775	2830063	13.85%	3.212%
8	15.992	2187	2194	2212	rBV	4743795	6554606	32.08%	7.440%
9	17.245	2401	2407	2413	rBV	2319351	3182988	15.58%	3.613%
10	18.145	2555	2560	2569	rBV	603643	867751	4.25%	0.985%
11	19.868	2848	2853	2862	rBV	10136346	11971250	58.58%	13.588%
12	21.145	3065	3070	3079	rBV	1589783	2155369	10.55%	2.447%
13	21.421	3113	3117	3125	rBV	2676825	3423240	16.75%	3.886%
14	23.786	3513	3519	3528	rVB2	1760807	3518436	17.22%	3.994%
15	26.221	3927	3933	3948	rVB2	612621	1916439	9.38%	2.175%
16	26.509	3970	3982	4000	rVB2	6606074	20434533	100.00%	23.195%
17	27.068	4071	4077	4085	rVB4	711990	1833525	8.97%	2.081%

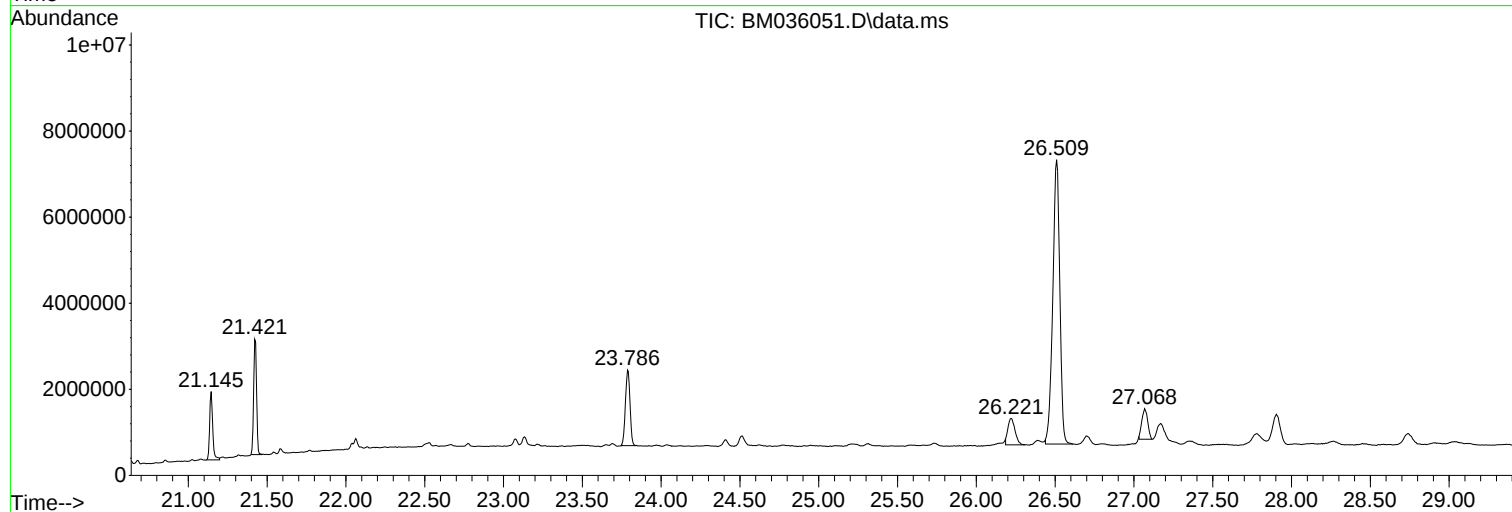
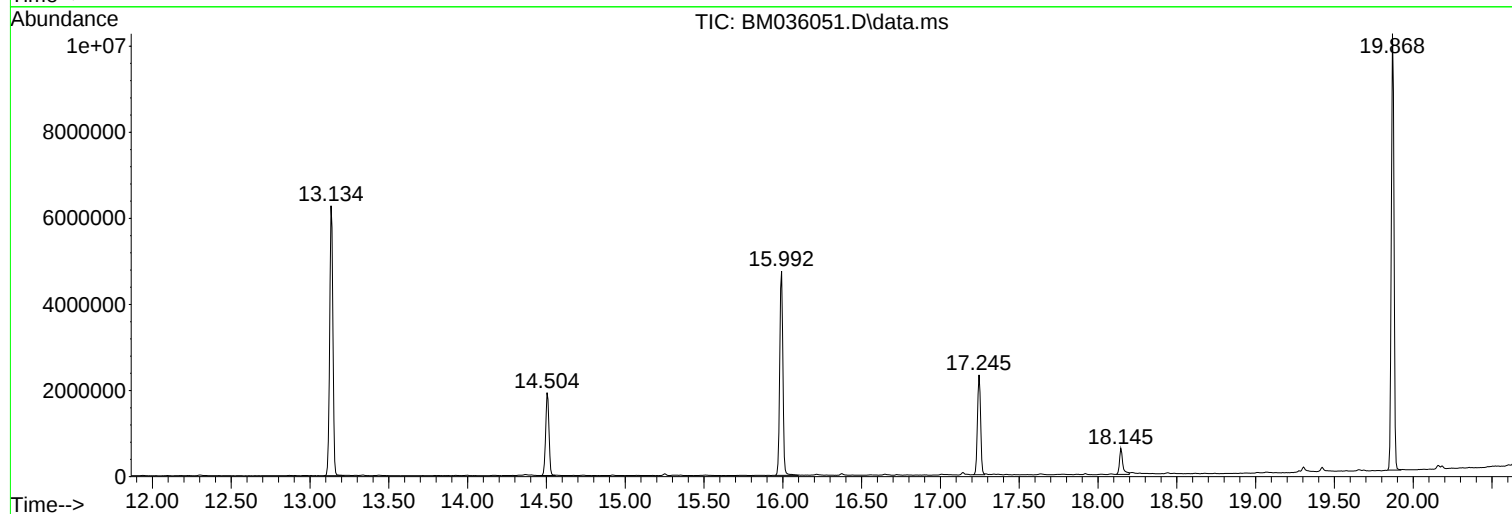
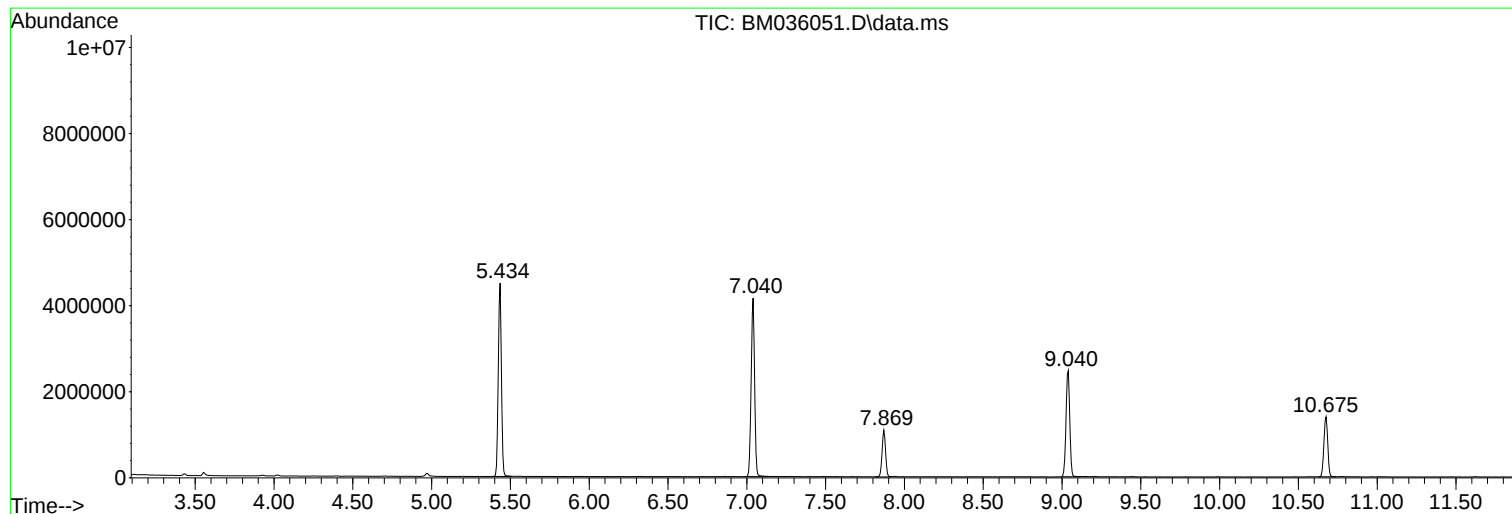
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM080122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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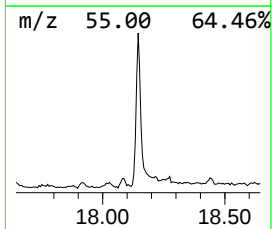
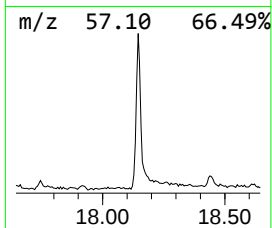
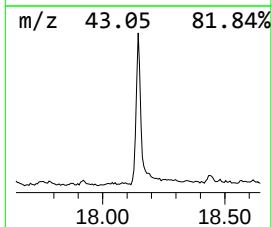
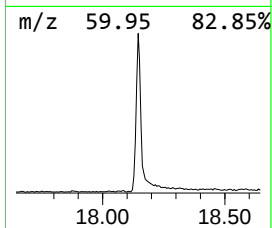
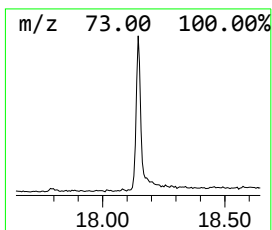
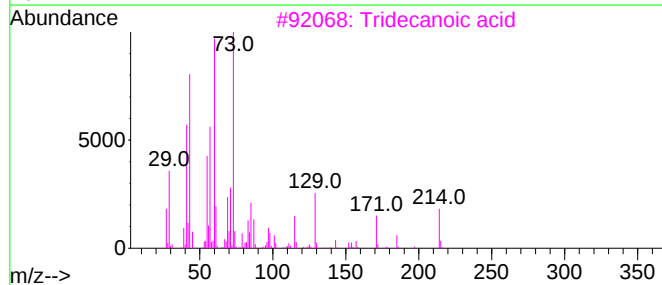
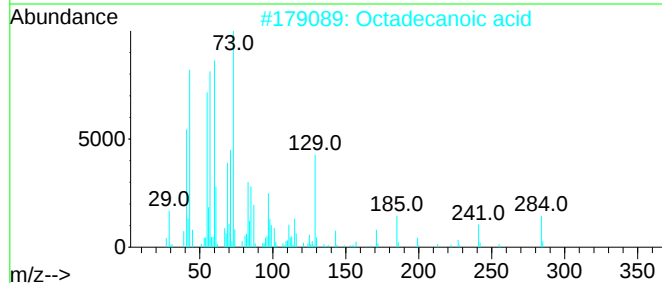
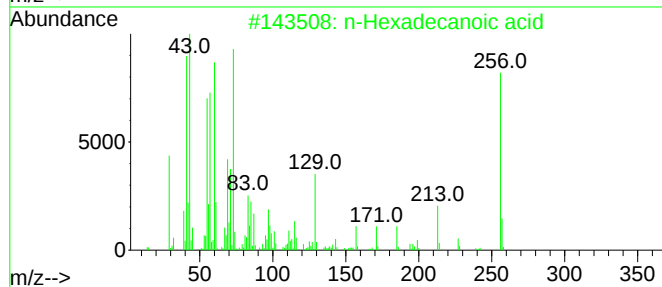
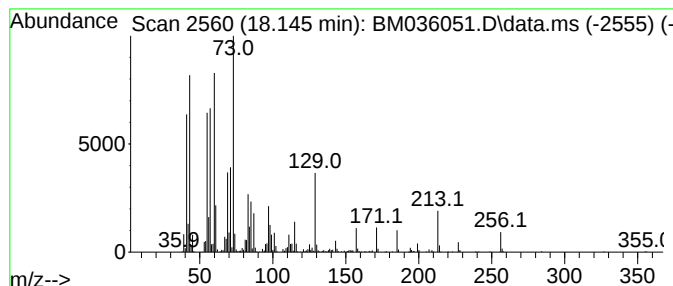
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	5.45 ng	867751	Phenanthrene-d10	17.245

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Octadecanoic acid	284	C18H36O2	000057-11-4	83
3		Tridecanoic acid	214	C13H26O2	000638-53-9	81
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	76
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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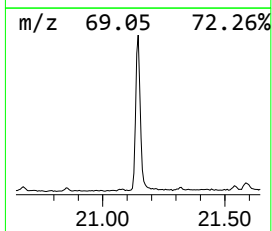
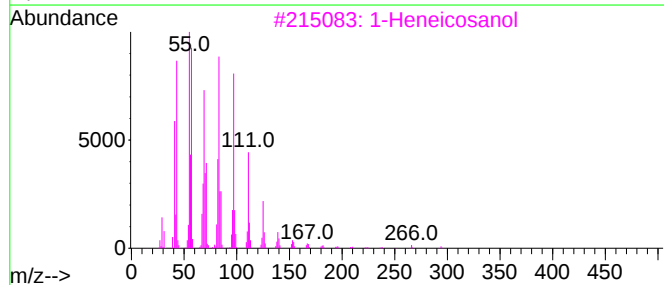
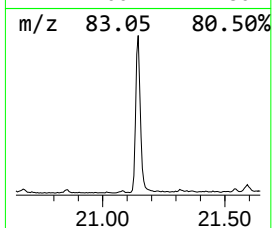
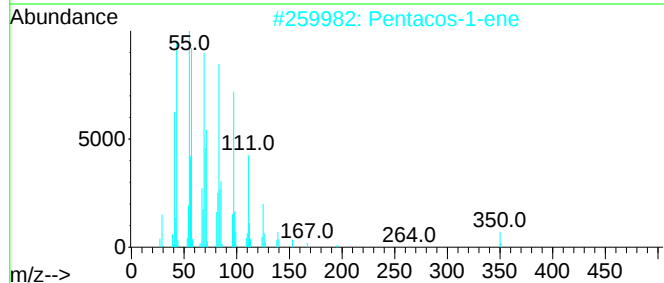
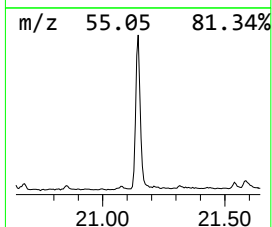
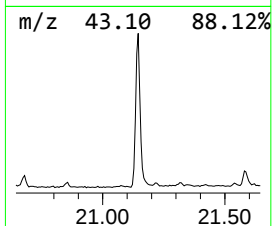
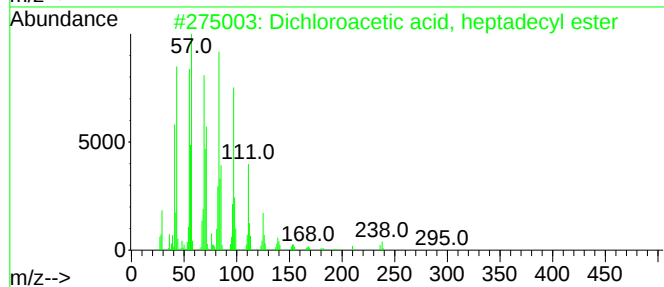
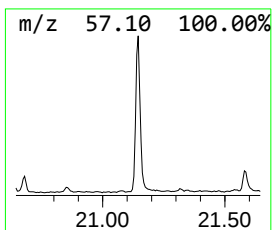
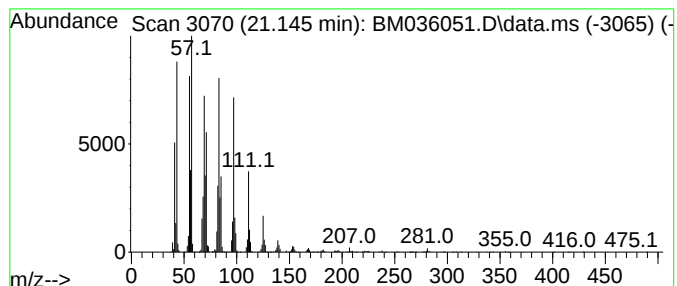
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Dichloroacetic acid, heptad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.145	12.59 ng	2155370	Chrysene-d12	21.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			1-Heneicosanol	312	C21H44O	015594-90-8	93
4			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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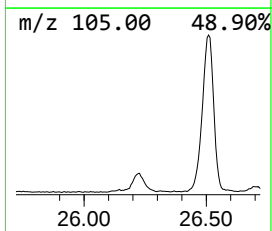
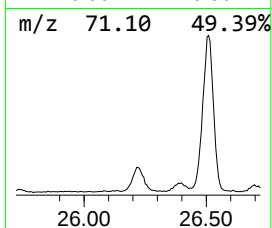
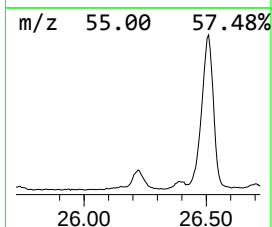
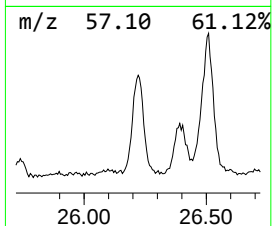
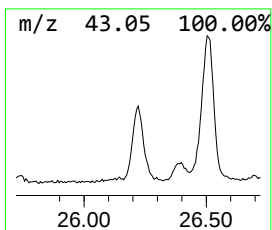
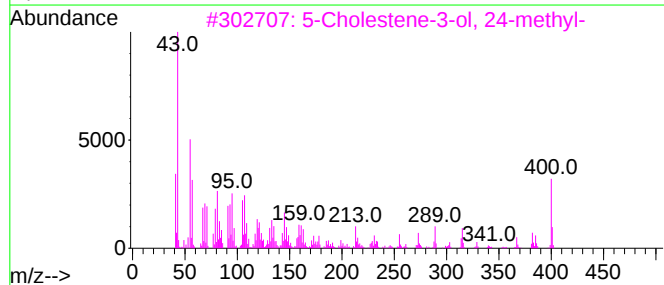
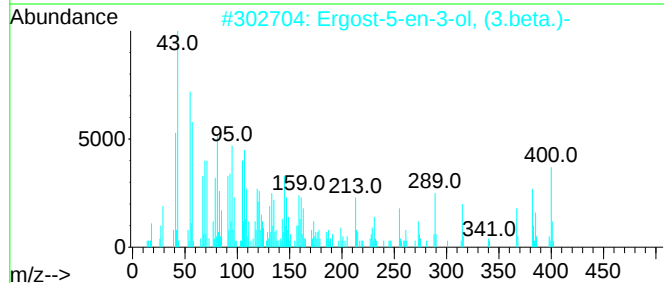
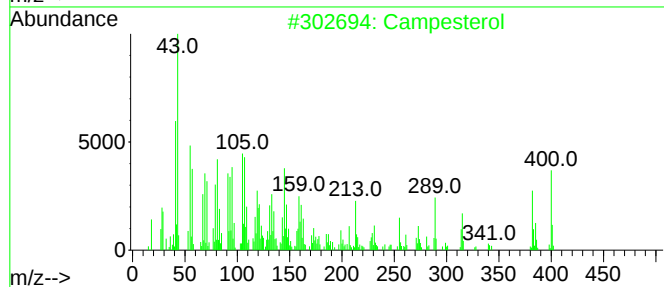
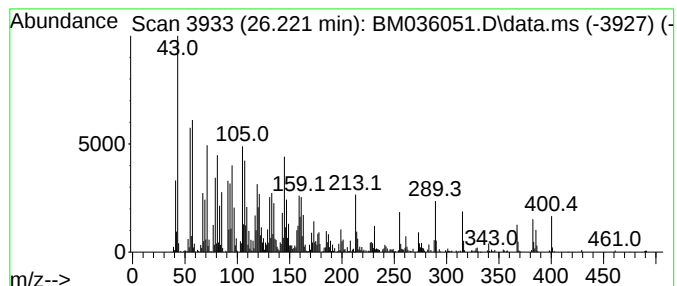
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Peak Number 3 Campesterol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.221	10.89 ng	1916440	Perylene-d12	23.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Campesterol	400	C28H48O	000474-62-4	96
2			Ergost-5-en-3-ol, (3.beta.)-	400	C28H48O	004651-51-8	95
3			5-Cholestene-3-ol, 24-methyl-	400	C28H48O	290299-12-6	95
4			Ergost-7-en-3-ol, (3.beta.)-	400	C28H48O	026047-31-4	86
5			Cholest-5-ene, 3-methoxy-, (3.be...	400	C28H48O	001174-92-1	86



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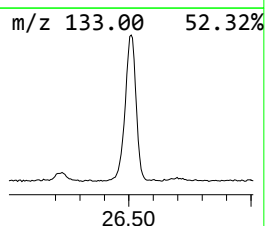
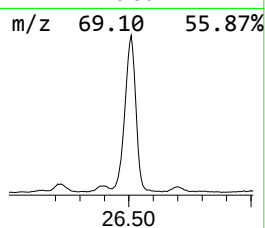
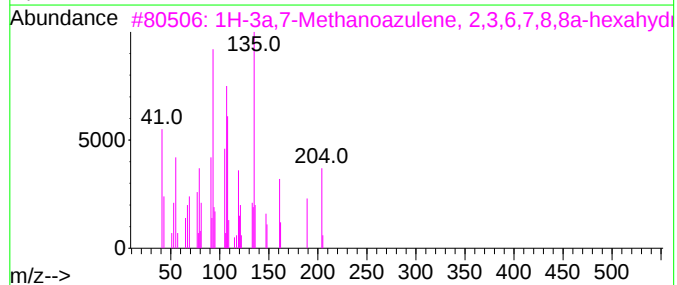
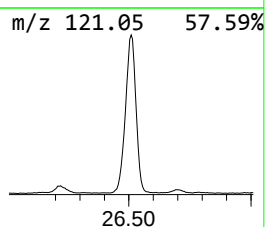
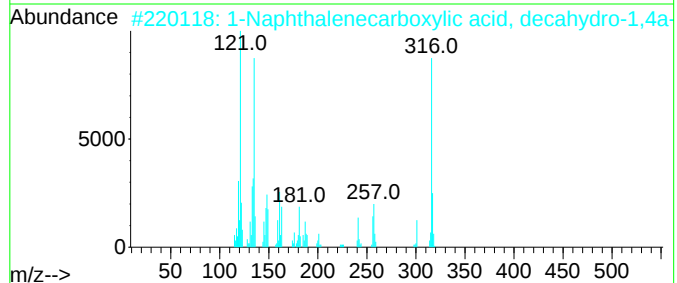
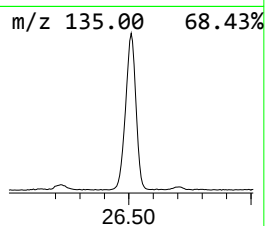
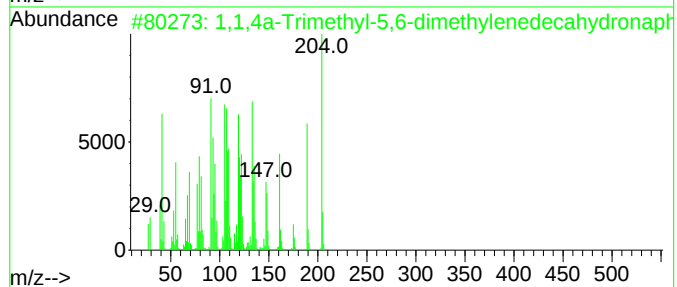
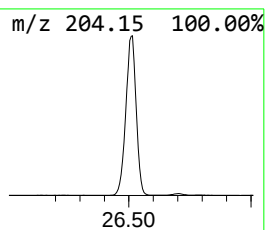
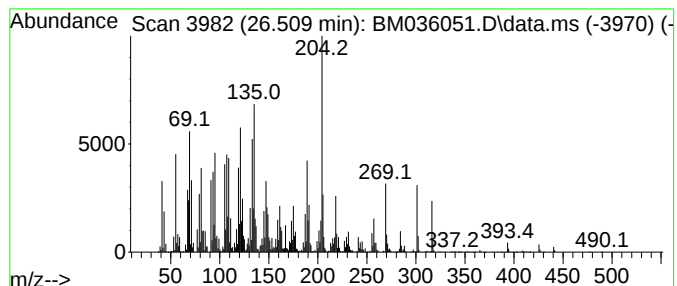
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Peak Number 4 1,1,4a-Trimethyl-5,6-dimeth... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
26.509	116.16 ng	20434500	Perylene-d12	23.786	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,4a-Trimethyl-5,6-dimethylene...	204	C15H24	1000193-60-8	62
2	1-Naphthalenecarboxylic acid, de...	316	C21H32O2	001235-39-8	49
3	1H-3a,7-Methanoazulene, 2,3,6,7,...	204	C15H24	000560-32-7	49
4	1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1010140-07-7	49
5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	46



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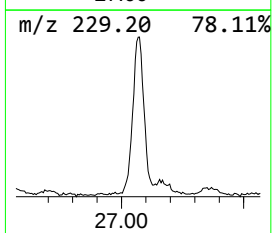
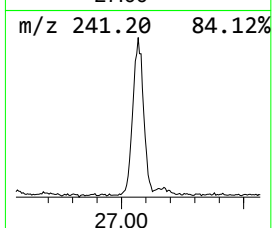
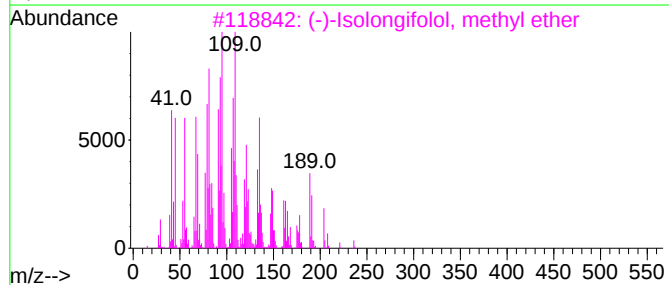
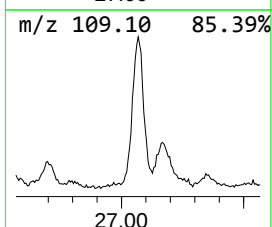
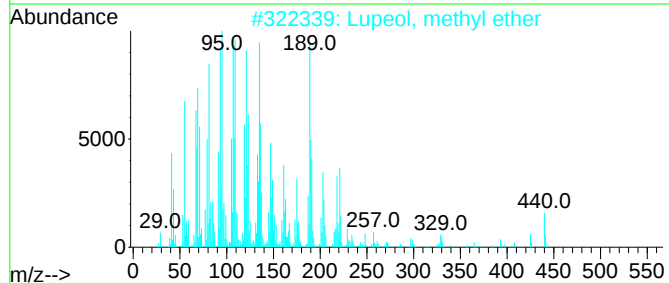
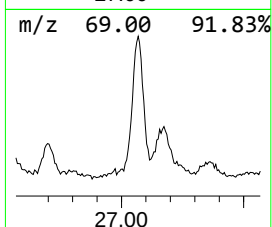
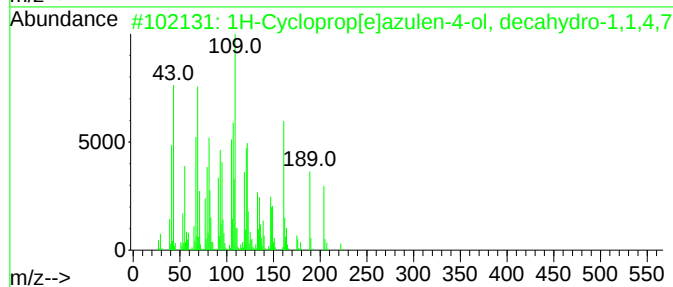
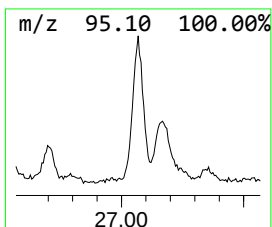
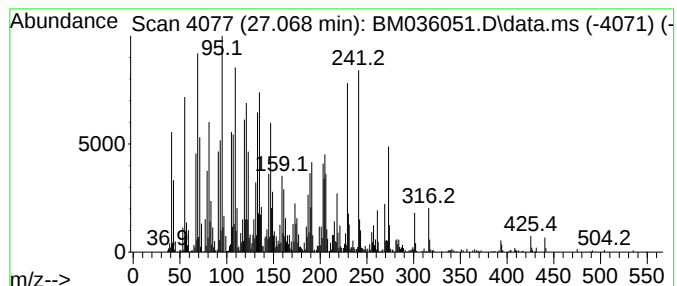
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Peak Number 5 unknown27.068 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.068	10.42 ng	1833530	Perylene-d12	23.786

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	46
2			Lupeol, methyl ether	440	C31H52O	025279-38-3	38
3			(-)-Isolongifolol, methyl ether	236	C16H28O	1000333-80-8	35
4			(1R,4aR,5S)-5-((E)-5-Methoxy-3-m...	318	C21H34O2	1000495-78-7	30
5			4-(1,3,3-Trimethyl-bicyclo[4.1.0...	206	C14H22O	077143-31-8	25



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.145	5.5	ng	867751	4	17.245	3182990	20.0
Dichloroacetic ...	21.145	12.6	ng	2155370	5	21.427	3423240	20.0
Campesterol	26.221	10.9	ng	1916440	6	23.786	3518440	20.0
1,1,4a-Trimethy...	26.509	116.2	ng	20434500	6	23.786	3518440	20.0
unknown27.068	27.068	10.4	ng	1833530	6	23.786	3518440	20.0