

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF061818\
 Data File : BF106536.D
 Acq On : 18 Jun 2018 14:12
 Operator : JU/SJ
 Sample : J3502-01
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180367-SITE-WATER

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BF061118.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.196	483	486	494	rBV	75981	84610	2.55%	0.345%
2	5.607	553	556	564	rBV	1692525	1622172	48.85%	6.609%
3	6.607	722	726	732	rBV	1247093	1206581	36.34%	4.916%
4	6.742	745	749	752	rBV	2636085	2473038	74.47%	10.076%
5	6.966	783	787	790	rBV	939690	751069	22.62%	3.060%
6	7.125	809	814	817	rBV	2411953	2294567	69.10%	9.349%
7	7.531	877	883	886	rBV	1962868	1984751	59.77%	8.086%
8	8.248	1001	1005	1008	rBV	1113808	937769	28.24%	3.821%
9	9.325	1183	1188	1191	rBV	3356645	3297559	99.30%	13.435%
10	9.713	1250	1254	1259	rBV	273614	228791	6.89%	0.932%
11	9.919	1285	1289	1293	rBV	53927	44009	1.33%	0.179%
12	10.007	1300	1304	1311	rVB	1210075	1039524	31.30%	4.235%
13	10.419	1372	1374	1377	rVB2	86619	65139	1.96%	0.265%
14	10.666	1413	1416	1419	rVB	354314	285096	8.59%	1.162%
15	10.801	1434	1439	1442	rBV	2200200	2087212	62.86%	8.504%
16	10.895	1452	1455	1465	rVB	67690	82439	2.48%	0.336%
17	11.495	1554	1557	1561	rBV	1126268	1063921	32.04%	4.335%
18	13.089	1823	1828	1831	rBV	3177258	3320660	100.00%	13.529%
19	13.971	1974	1978	1984	rBV	84348	100808	3.04%	0.411%
20	14.154	2005	2009	2013	rBV	900143	804943	24.24%	3.280%
21	15.024	2153	2157	2161	rBV2	119174	123051	3.71%	0.501%
22	15.701	2267	2272	2285	rVB	482760	646597	19.47%	2.634%

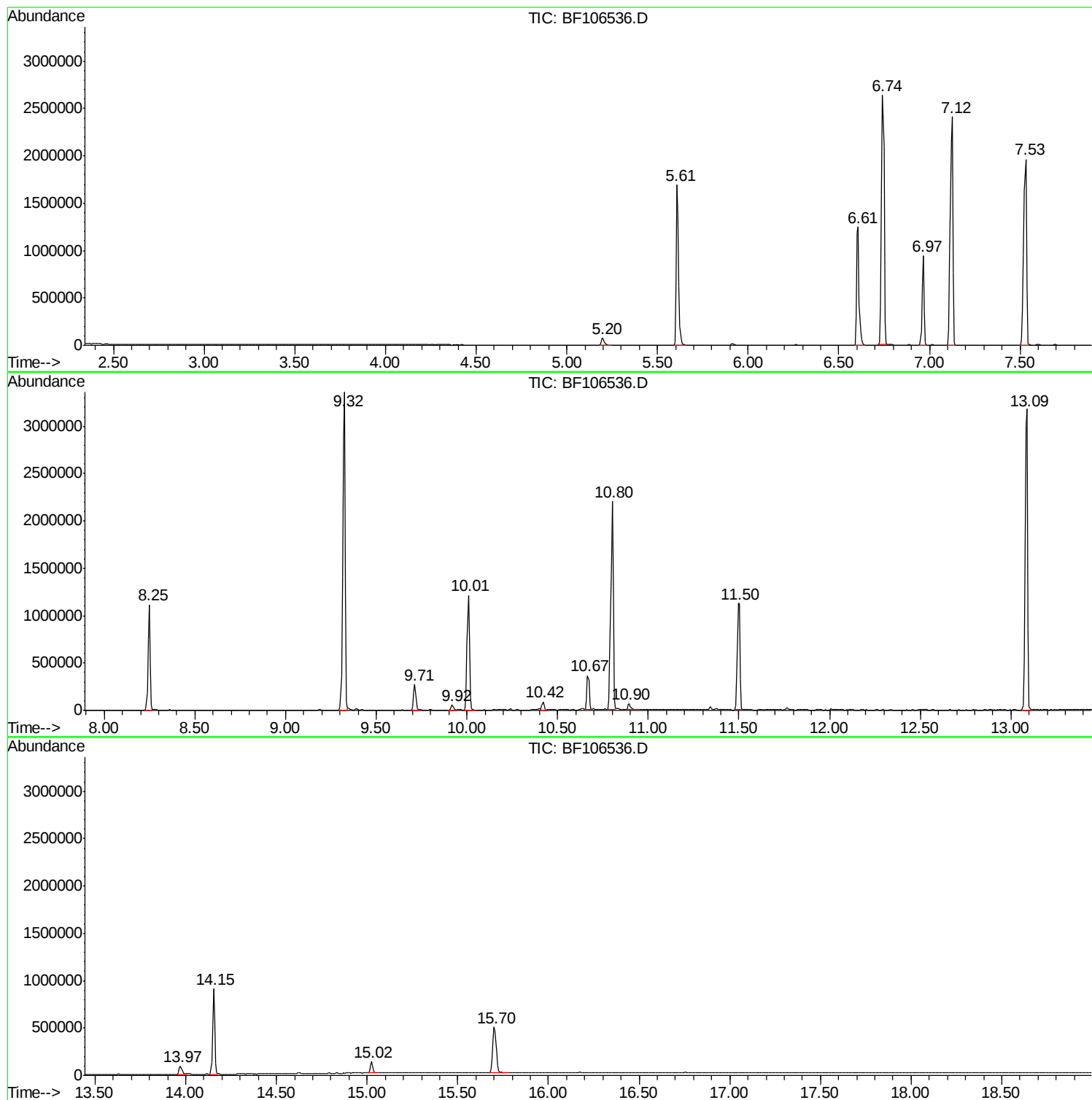
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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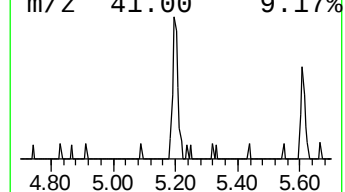
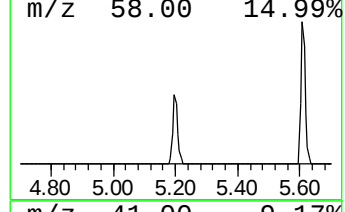
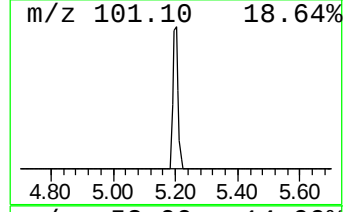
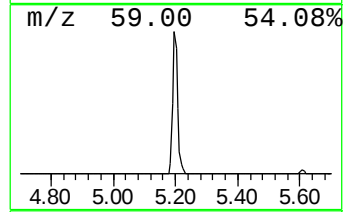
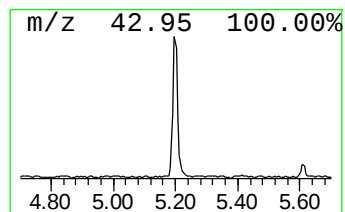
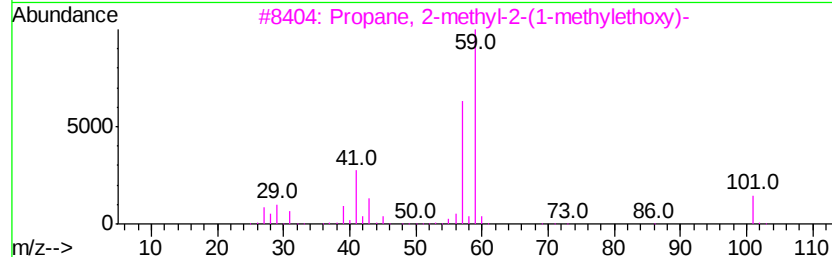
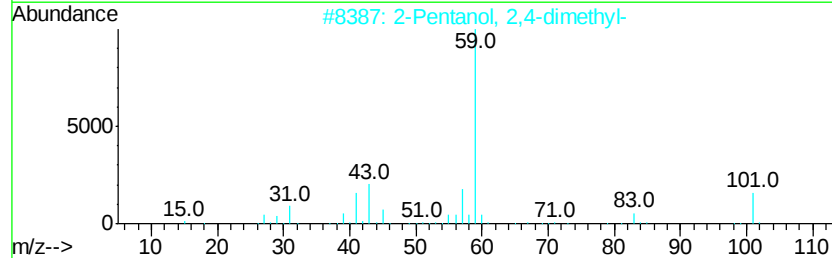
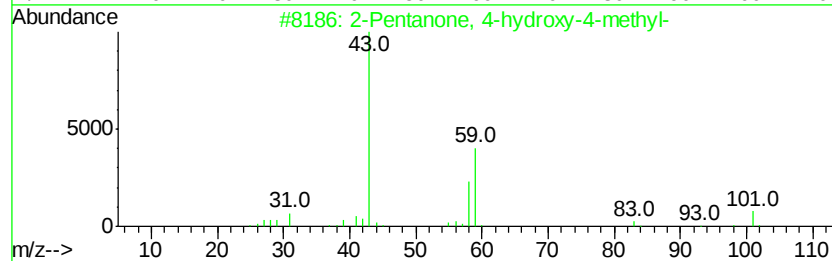
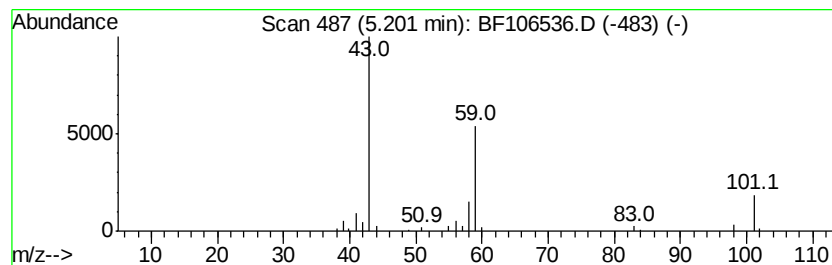
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.25 ng	84610	1,4-Dichlorobenzene-d4	6.97

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	42
3			Propane, 2-methyl-2-(1-methylethoxy)-	116	C7H16O	017348-59-3	36
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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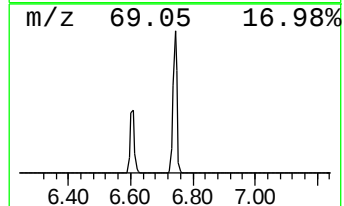
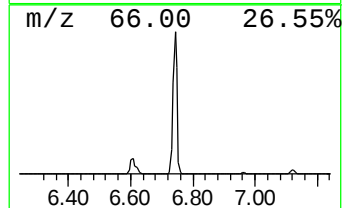
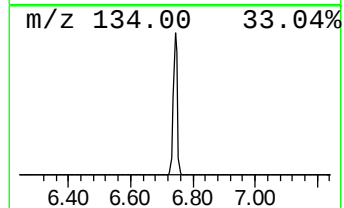
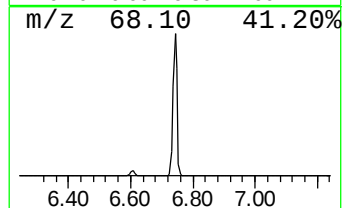
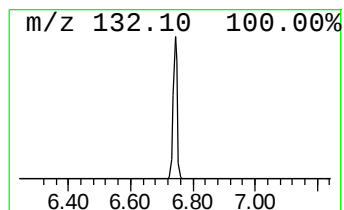
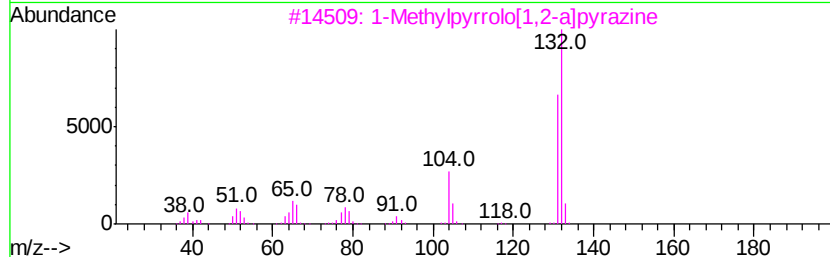
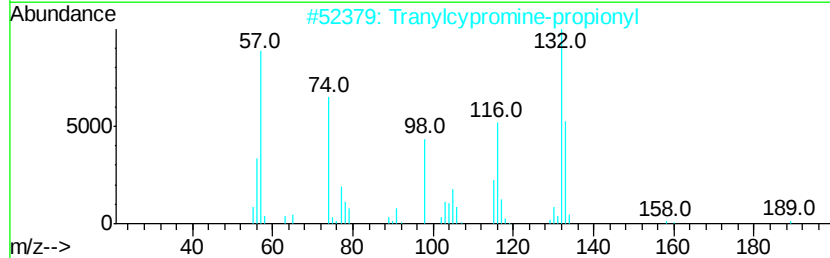
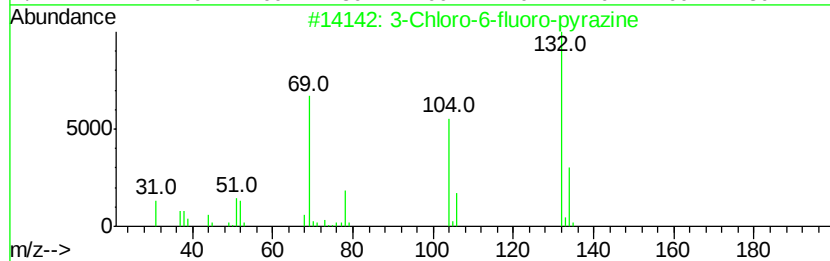
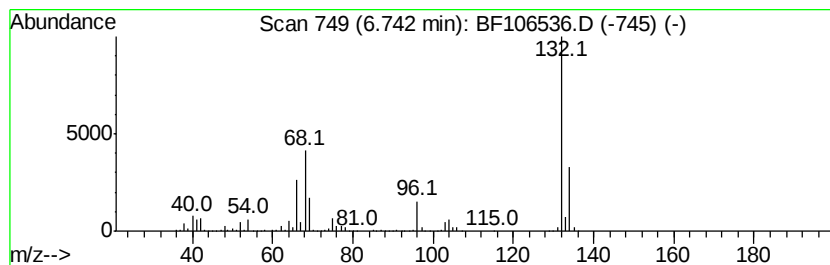
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	65.85 ng	2473040	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9



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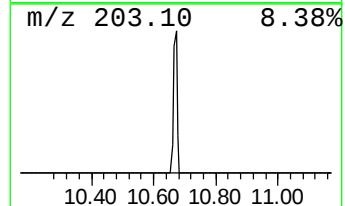
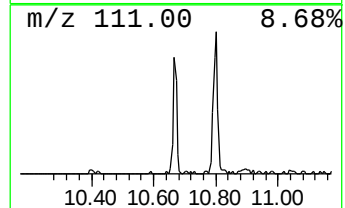
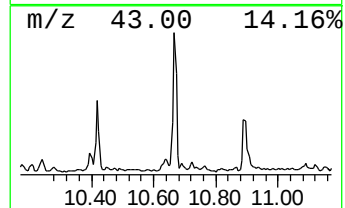
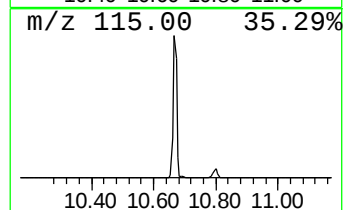
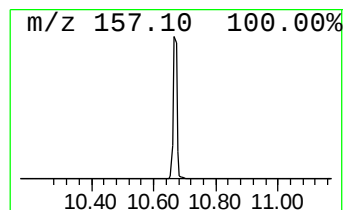
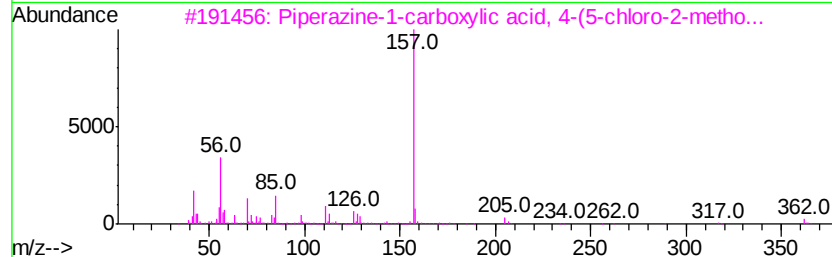
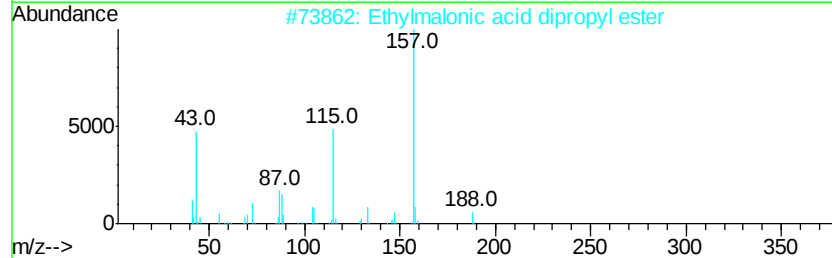
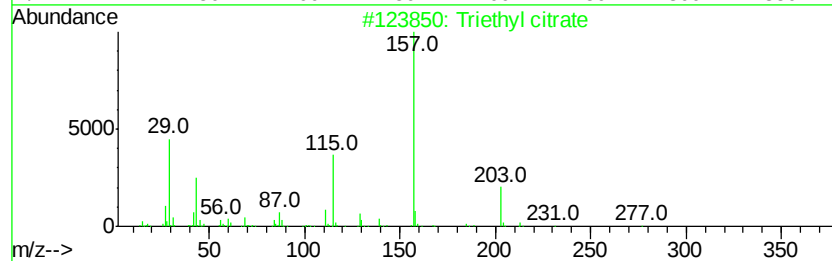
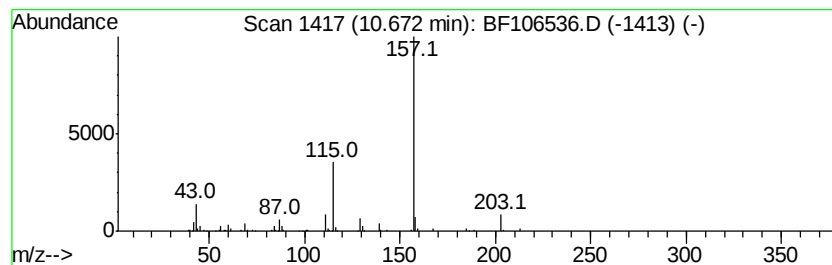
Instrument :
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Peak Number 4 Triethyl citrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.67	5.49 ng	285096	Acenaphthene-d10	10.01
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Triethyl citrate	276 C12H20O7	000077-93-0 91
2		Ethylmalonic acid dipropyl ester	216 C11H20O4	001113-91-3 64
3		Piperazine-1-carboxylic acid, 4-...	362 C14H19ClN2O5S	1000303-80-2 38
4		2-Chlorobenzoic acid, pentadecyl...	366 C22H35ClO2	1000292-43-0 38
5		N-Methoxy-2,2-dicarbomethoxyazir...	189 C7H11NO5	053084-34-7 32



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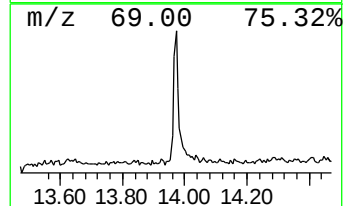
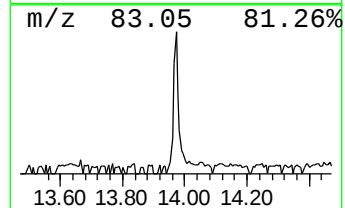
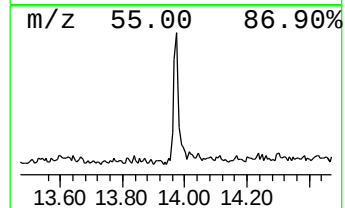
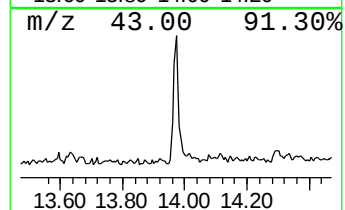
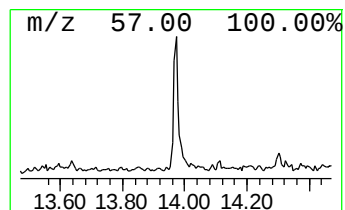
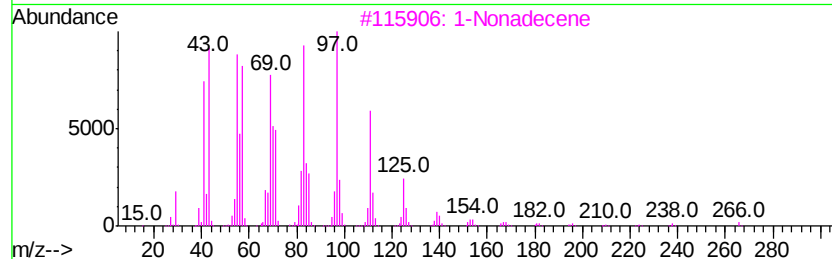
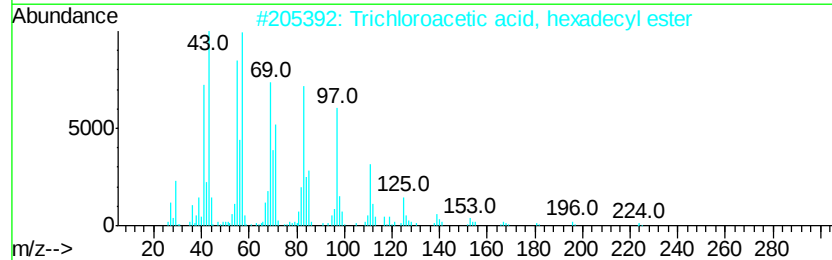
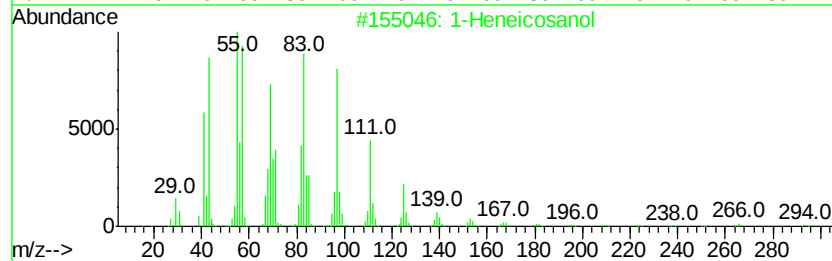
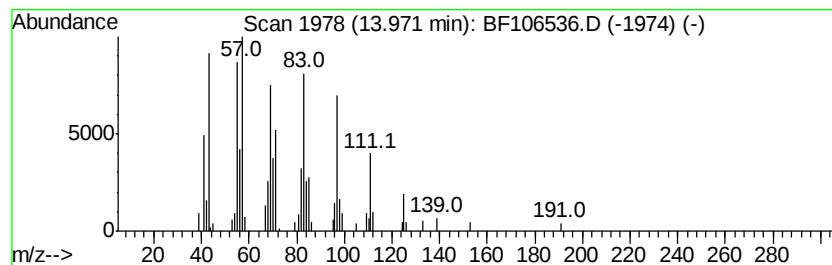
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	2.50 ng	100808	Chrysene-d12	14.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91
3		1-Nonadecene	266	C19H38	018435-45-5	91
4		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
5		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91



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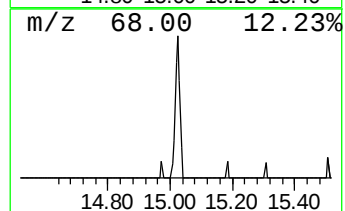
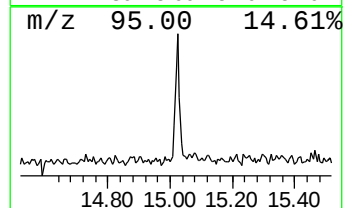
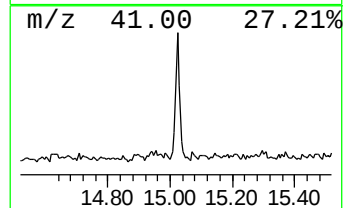
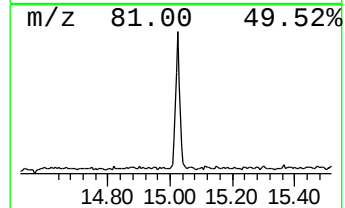
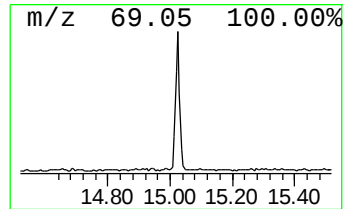
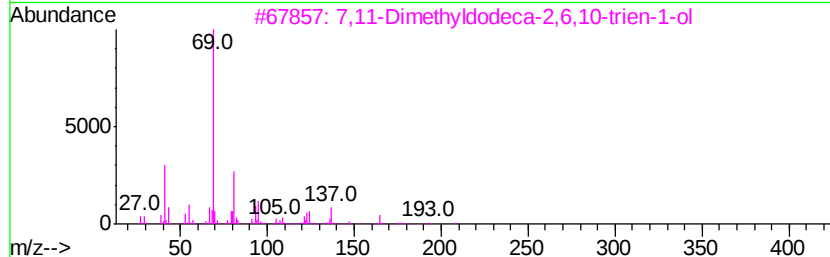
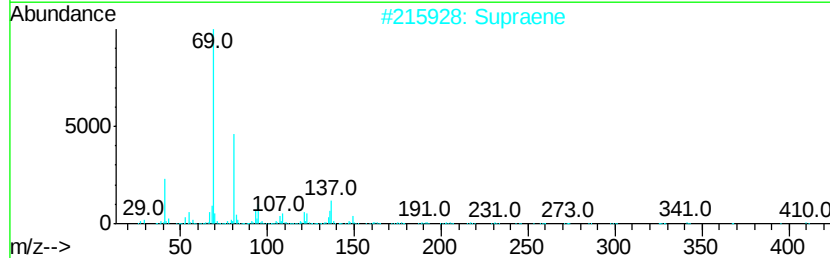
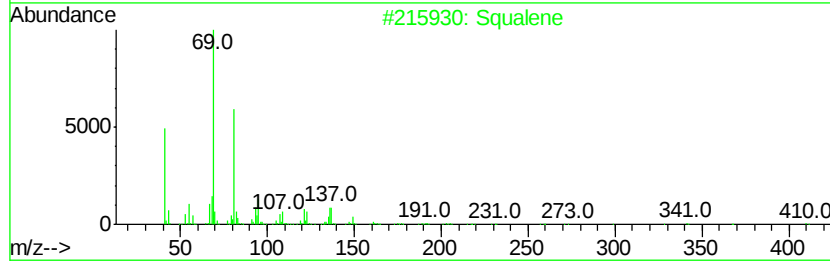
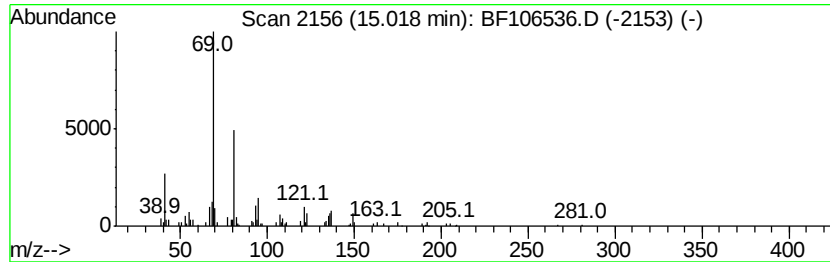
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.02	3.81 ng	123051	Perylene-d12	15.70

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			Supraene	410	C30H50	007683-64-9	83
3			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	68
4			(.+/-)-Lavandulol, pentafluorop...	300	C13H17F5O2	1000352-63-1	64
5			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	2.3	ng	84610	1	6.97	751069	20.0
unknown6.74	6.74	65.8	ng	2473040	1	6.97	751069	20.0
Triethyl citrate	10.67	5.5	ng	285096	3	10.01	1039520	20.0
1-Heneicosanol	13.97	2.5	ng	100808	5	14.15	804943	20.0
Squalene	15.02	3.8	ng	123051	6	15.70	646597	20.0