

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062618\
 Data File : BF106836.D
 Acq On : 26 Jun 2018 21:12
 Operator : JU/SJ
 Sample : J3570-01
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20180371-COMPOSITE-CS-1A

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-BF061918.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	5.201	484	487	495	rBV	48388	58836	6.93%	0.739%
2	5.607	552	556	569	rBV	784448	756686	89.06%	9.500%
3	6.607	722	726	744	rBV	787010	781434	91.97%	9.811%
4	6.742	744	749	752	rBV	829586	775902	91.32%	9.742%
5	6.960	783	786	790	rBB	303697	239660	28.21%	3.009%
6	7.119	809	813	816	rBV	754087	621100	73.10%	7.798%
7	7.525	877	882	885	rBV	520905	475600	55.98%	5.971%
8	8.242	1001	1004	1009	rBV	307897	271571	31.96%	3.410%
9	9.319	1183	1187	1195	rVB	771580	717366	84.43%	9.007%
10	9.707	1249	1253	1260	rBV	100349	95318	11.22%	1.197%
11	9.907	1284	1287	1291	rVB2	14884	14121	1.66%	0.177%
12	10.001	1300	1303	1311	rVB	290657	277233	32.63%	3.481%
13	10.413	1370	1373	1375	rVB2	17817	16045	1.89%	0.201%
14	10.630	1406	1410	1413	rBV	11339	13976	1.64%	0.175%
15	10.795	1435	1438	1442	rBV	459949	437961	51.55%	5.499%
16	10.883	1450	1453	1459	rBV2	15947	23984	2.82%	0.301%
17	11.360	1532	1534	1545	rVB4	11787	16278	1.92%	0.204%
18	11.495	1554	1557	1561	rBV	330969	296327	34.88%	3.721%
19	12.671	1753	1757	1758	rBV4	23823	35418	4.17%	0.445%
20	12.995	1809	1812	1814	rBV3	55477	68947	8.12%	0.866%
21	13.077	1823	1826	1833	rVB	844440	849617	100.00%	10.667%
22	13.812	1948	1951	1964	rVB2	185317	575233	67.70%	7.222%
23	14.148	2005	2008	2011	rBV	357926	341110	40.15%	4.283%
24	15.689	2268	2270	2277	rVB	150855	204985	24.13%	2.574%

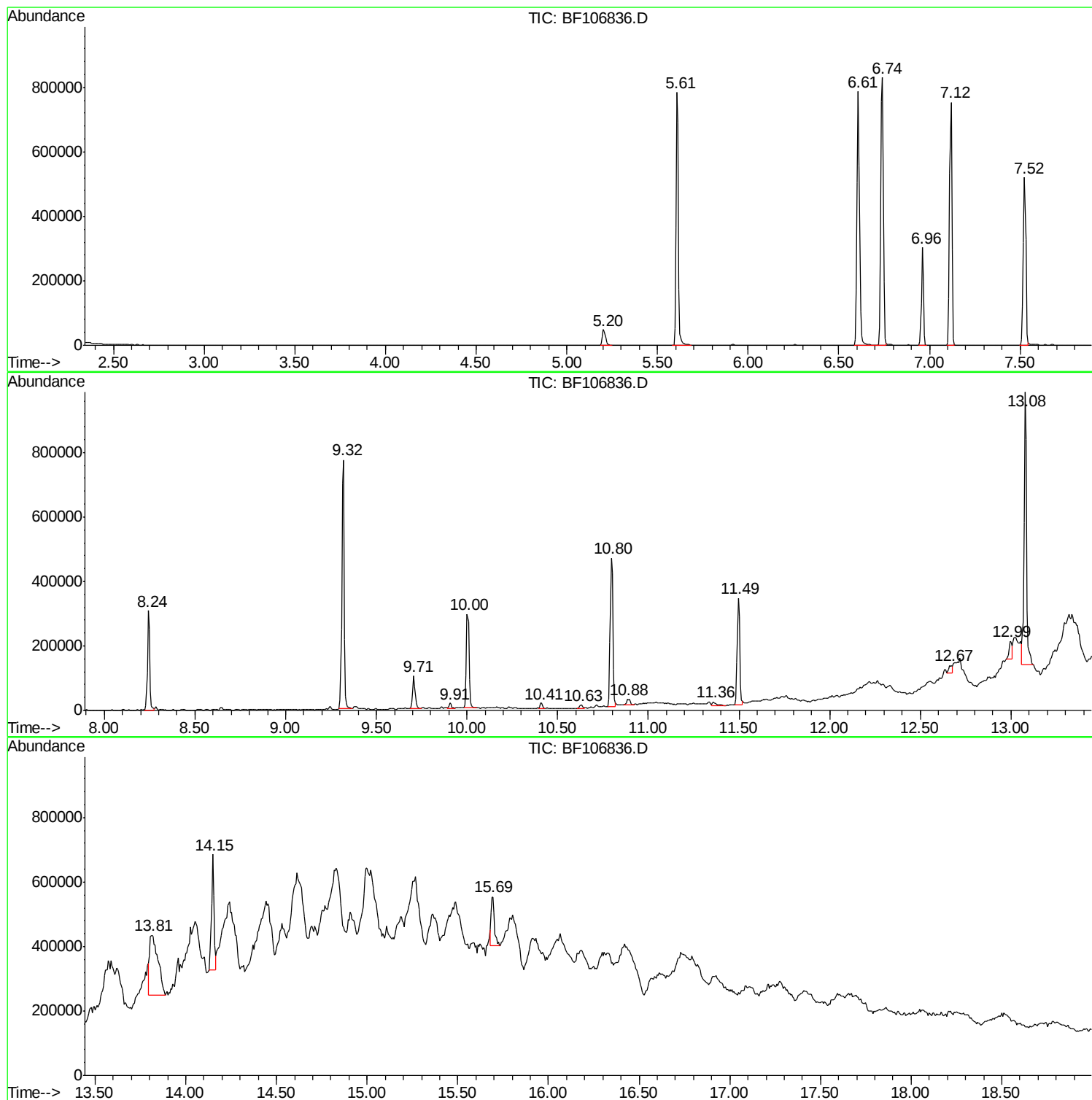
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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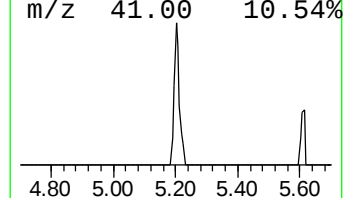
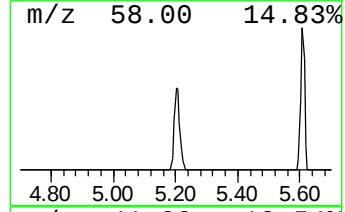
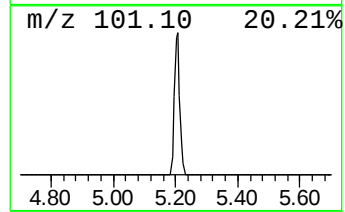
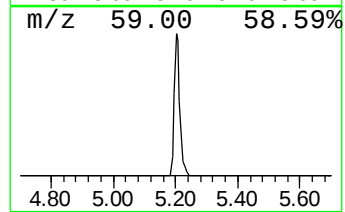
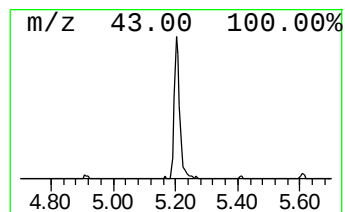
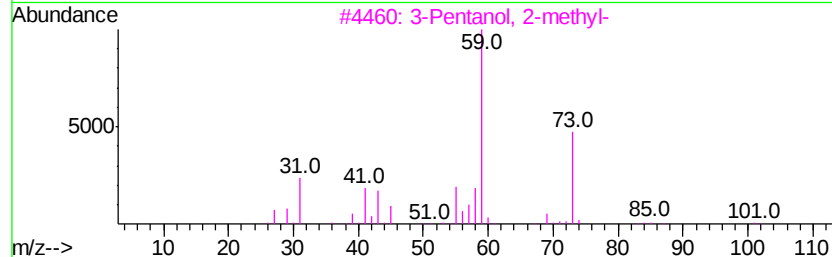
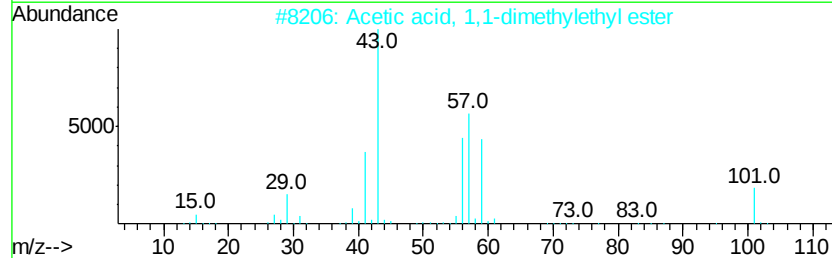
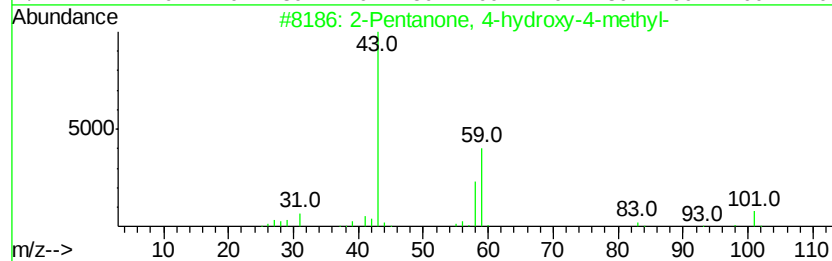
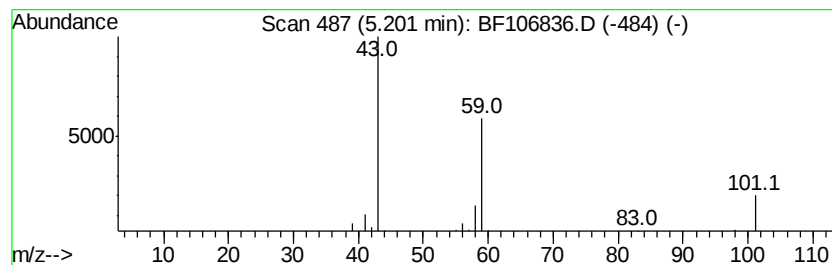
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	4.91 ng	58836	1,4-Dichlorobenzene-d4	6.96

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			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	9
4			3-Pentanol	88	C5H12O	000584-02-1	9
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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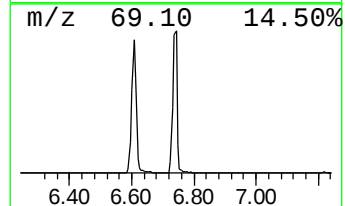
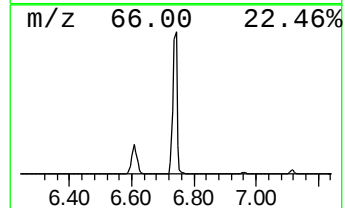
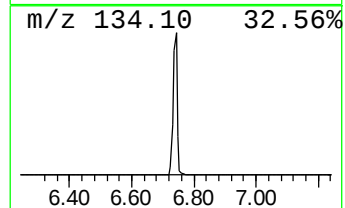
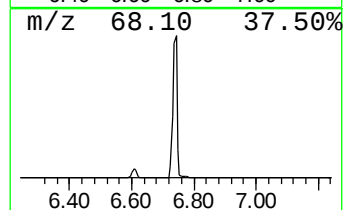
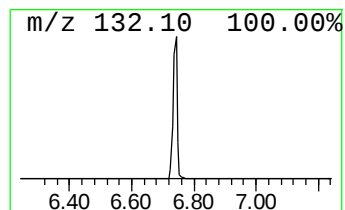
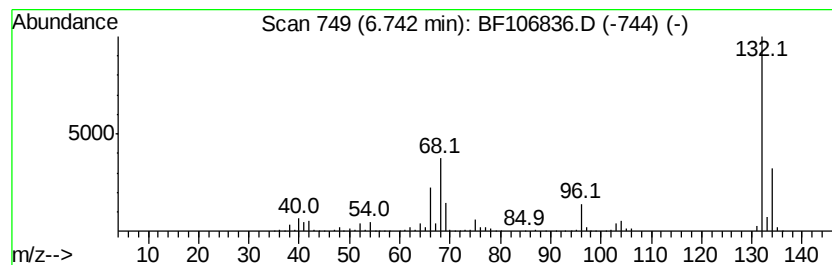
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	64.75 ng	775902	1,4-Dichlorobenzene-d4	6.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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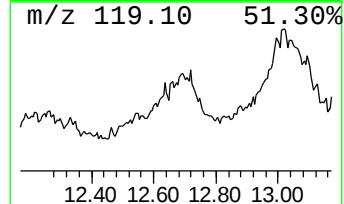
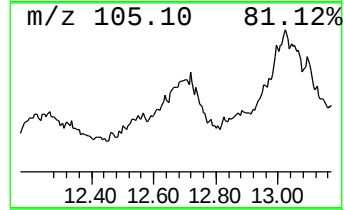
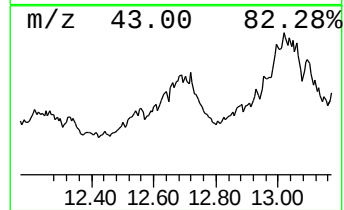
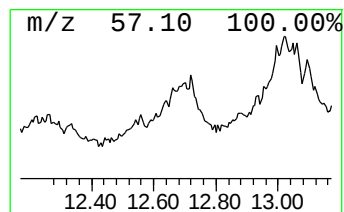
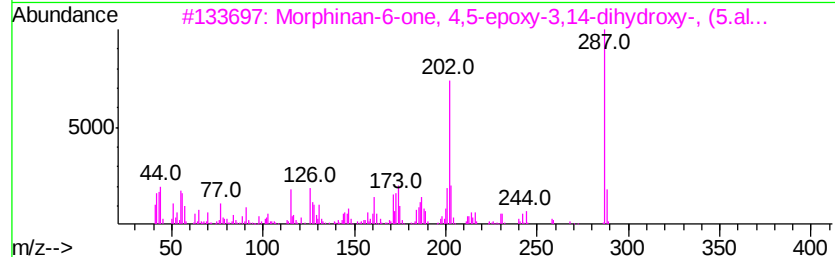
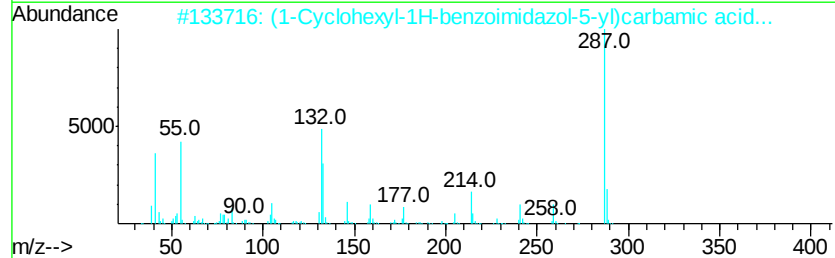
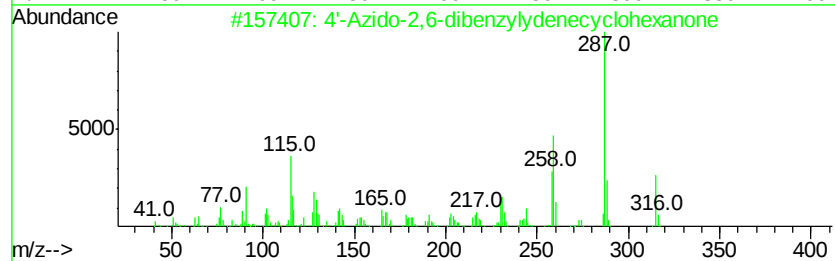
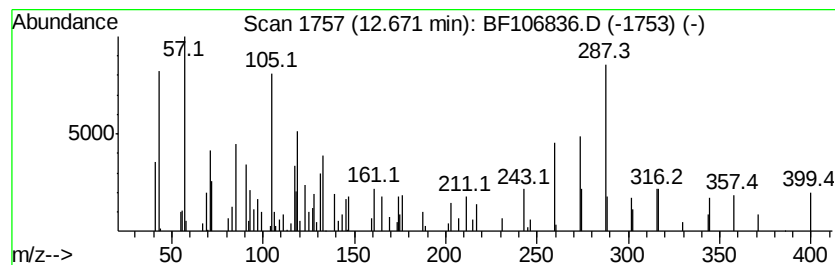
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Peak Number 4 unknown12.67 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.67	2.39 ng	35418	Phenanthrene-d10	11.49	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4'-Azido-2,6-dibenzylidenecyclohexanone	315	C20H17N3O	1000110-97-2	27
2	(1-Cyclohexyl-1H-benzimidazol-5-yl)carbamic acid	287	C16H21N3O2	1000310-00-5	22
3	Morphinan-6-one, 4,5-epoxy-3,14-dihydroxy-, (5.alpha.)-	287	C16H17N04	033522-95-1	11
4	Morphinan-4-ol-6-one, 2-methoxy-	287	C17H21N03	084229-97-0	11
5	Desmethyl dihydrocodeine	287	C17H21N03	000845-69-2	10



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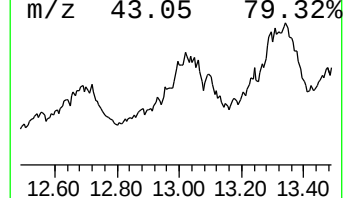
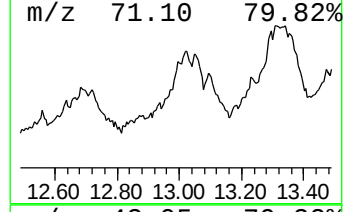
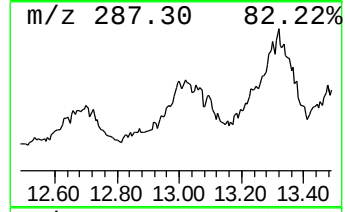
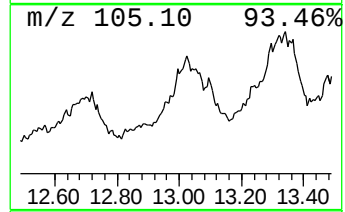
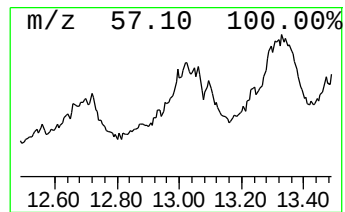
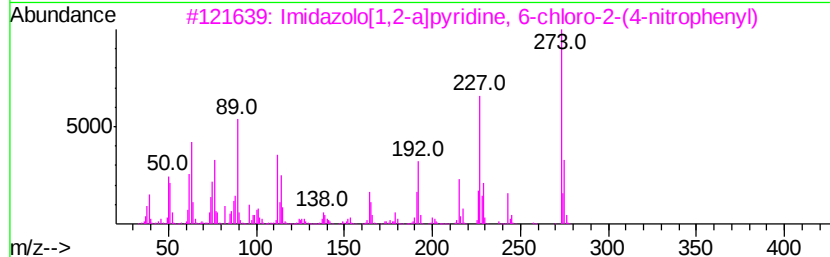
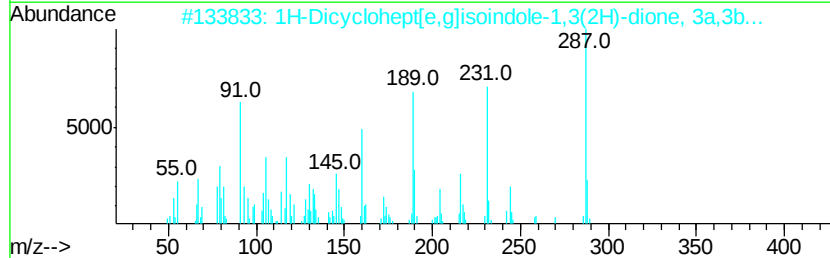
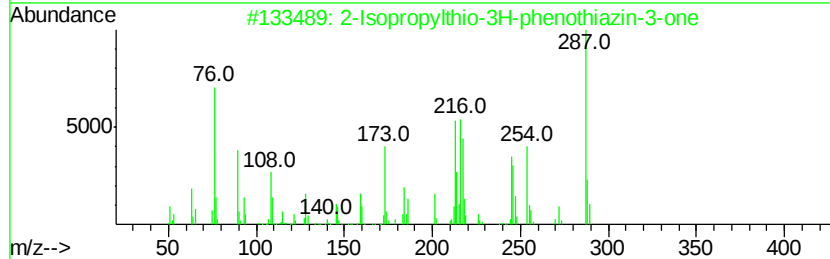
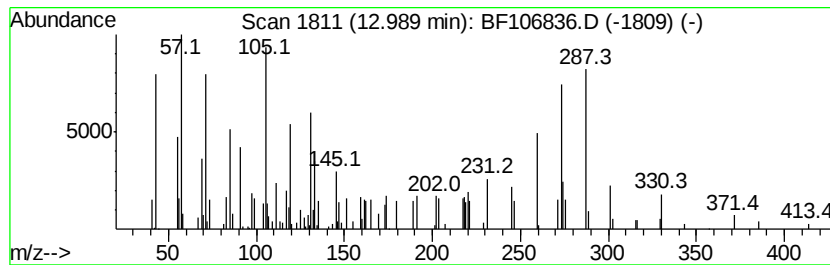
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown12.99 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.99	4.04 ng	68947	Chrysene-d12	14.15	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Isopropylthio-3H-phenothiazin-...	287	C15H13NOS2	090712-90-6	18
2	1H-Dicyclohept[e,g]isoindole-1,3...	287	C18H25N02	051624-46-5	18
3	Imidazolo[1,2-a]pyridine, 6-chlo...	273	C13H8ClN3O2	118000-62-7	15
4	2-Amino-4-[N-(4-butoxybenzyl)-N-m...	287	C15H21N5O	055384-22-0	14
5	17.alpha.-Hydroxy-11-desoxycorti...	388	C23H32O5	096391-56-9	14



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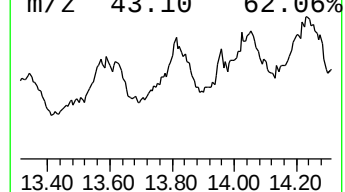
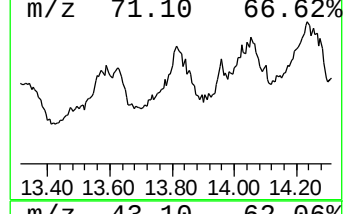
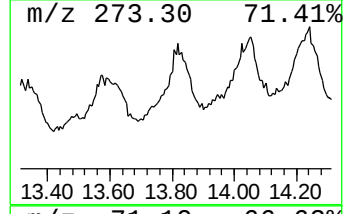
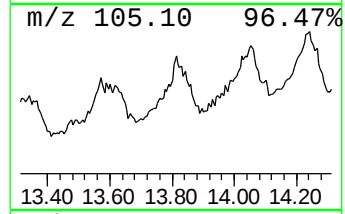
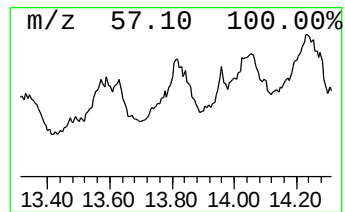
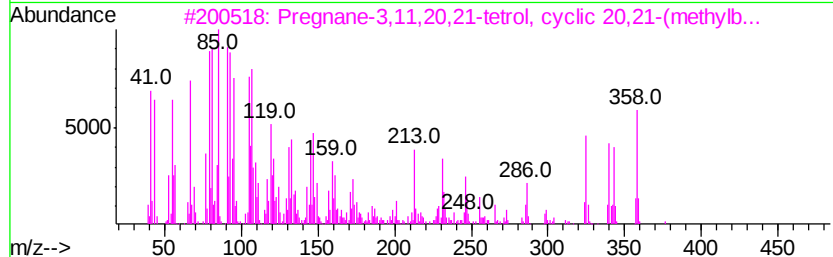
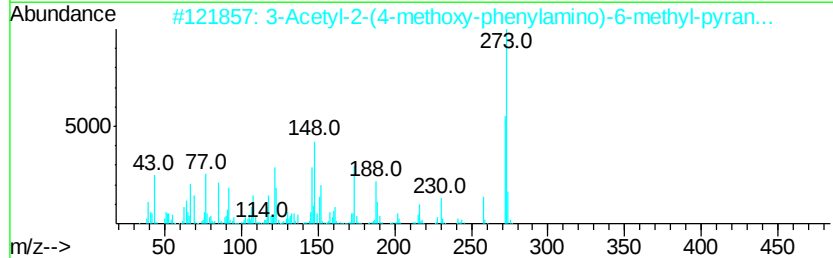
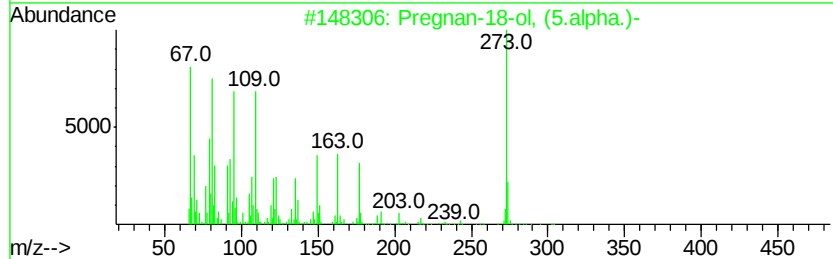
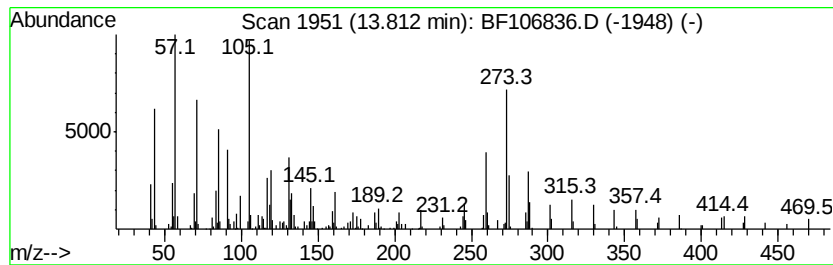
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 unknown13.81 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.		
13.81	33.73 ng	575233	Chrysene-d12		14.15		
Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pregnan-18-ol, (5.alpha.)-	304	C21H36O	056053-09-9	25
2			3-Acetyl-2-(4-methoxy-phenylamin...	273	C15H15NO4	1000300-68-2	25
3			Pregnane-3,11,20,21-tetrol, cvcl...	376	C22H37BO4	030882-72-5	11
4			Benzamide, N-(1,1'-biphenyl)-4-yl-	273	C19H15NO	020743-57-1	10
5			1H-Pyrazolo[3,4-b]quinoline, 3,6...	273	C18H15N3	1000302-05-0	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	4.9	ng	58836	1	6.96	239660	20.0
unknown6.74	6.74	64.8	ng	775902	1	6.96	239660	20.0
unknown12.67	12.67	2.4	ng	35418	4	11.49	296327	20.0
unknown12.99	12.99	4.0	ng	68947	5	14.15	341110	20.0
unknown13.81	13.81	33.7	ng	575233	5	14.15	341110	20.0