

Data Path : Z:\HPCHEM1\BNA F\DATA\BF022715\
 Data File : BF077510.D
 Acq On : 27 Feb 2015 17:37
 Operator : TP/IZ
 Sample : G1382-03
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW3-022515

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.550	55	58	61	rVB	354011	489491	20.92%	2.821%
2	1.595	61	62	70	rVV5	11659	37219	1.59%	0.214%
3	1.721	70	73	80	rVV	251917	373988	15.99%	2.155%
4	1.847	82	84	102	rVB	657408	1127426	48.19%	6.498%
5	5.036	361	363	369	rVB	99954	114463	4.89%	0.660%
6	5.550	405	408	410	rBV	659958	762548	32.59%	4.395%
7	6.807	516	518	521	rBV	324930	419642	17.94%	2.418%
8	6.967	529	532	534	rBV	1464403	1316724	56.28%	7.588%
9	7.253	555	557	560	rBV	344392	411603	17.59%	2.372%
10	7.447	571	574	576	rVB	1280297	1268976	54.24%	7.313%
11	7.950	615	618	620	rBV	1070017	987626	42.21%	5.692%
12	8.830	693	695	698	rBV	557767	562110	24.03%	3.240%
13	9.539	755	757	759	rBV	36188	30064	1.29%	0.173%
14	10.179	810	813	816	rBV	2394580	2067325	88.36%	11.914%
15	10.682	855	857	859	rVB	45081	36300	1.55%	0.209%
16	11.002	883	885	888	rBV	519125	659609	28.19%	3.801%
17	11.311	909	912	914	rBV	19117	26606	1.14%	0.153%
18	11.562	930	934	936	rBV2	25210	28782	1.23%	0.166%
19	11.905	962	964	966	rVB	67490	65733	2.81%	0.379%
20	11.985	969	971	974	rBV	1295315	1267793	54.19%	7.306%
21	12.854	1044	1047	1049	rBV	581189	715503	30.58%	4.124%
22	14.842	1219	1221	1224	rBV	1905197	2339548	100.00%	13.483%
23	16.031	1322	1325	1333	rBV	154073	246864	10.55%	1.423%
24	16.157	1333	1336	1338	rBV	616397	853041	36.46%	4.916%
25	16.877	1396	1399	1402	rBV4	15336	27727	1.19%	0.160%
26	17.288	1432	1435	1440	rBV5	8337	26155	1.12%	0.151%
27	17.963	1491	1494	1497	rBV	746498	941215	40.23%	5.424%
28	18.603	1548	1550	1555	rVB3	30427	56917	2.43%	0.328%
29	20.477	1711	1714	1719	rVB3	34544	90629	3.87%	0.522%

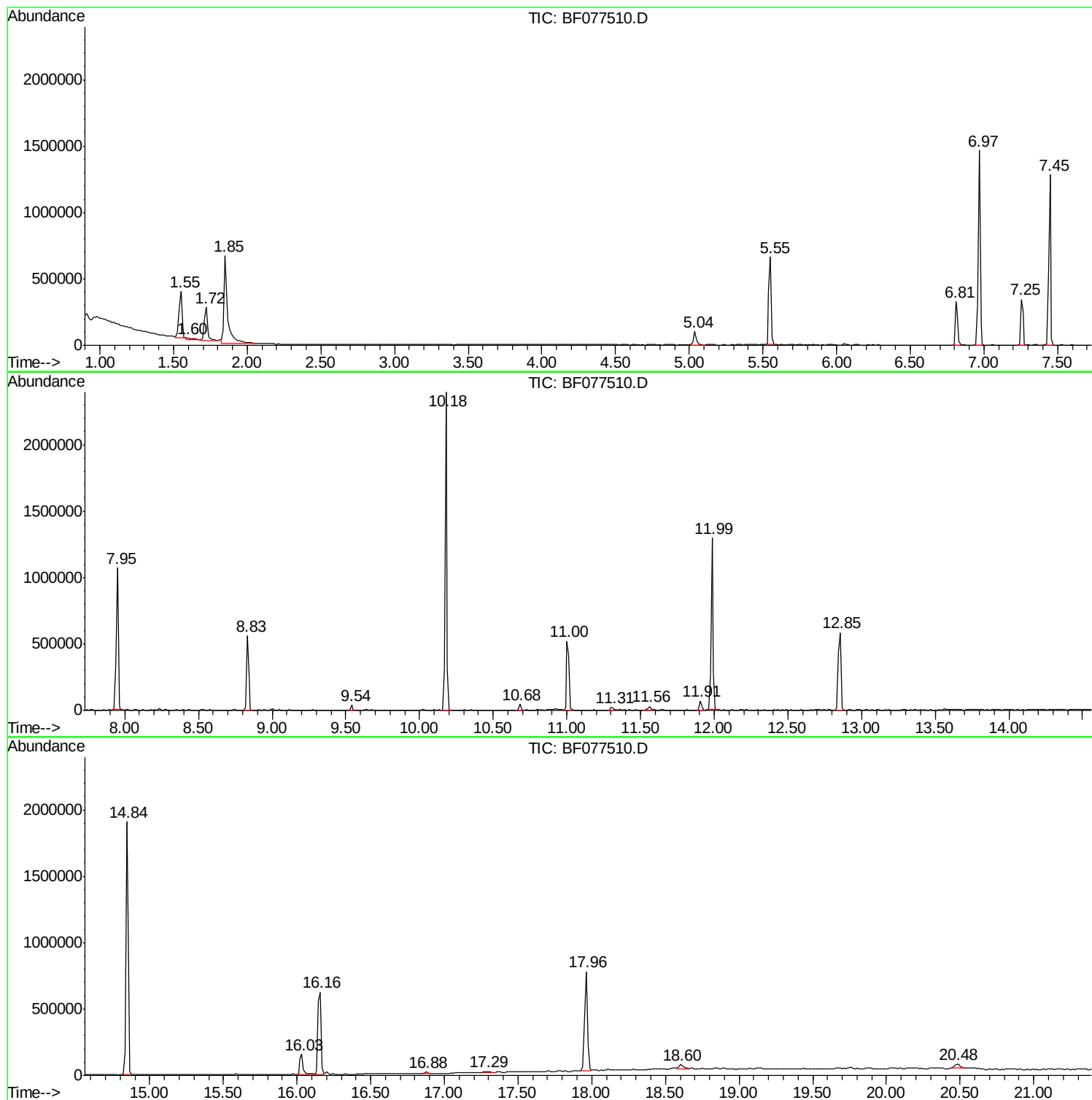
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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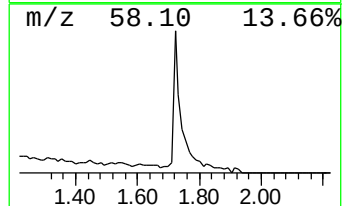
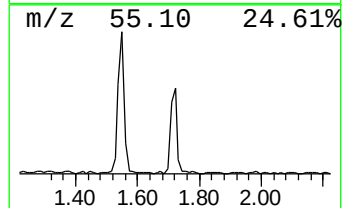
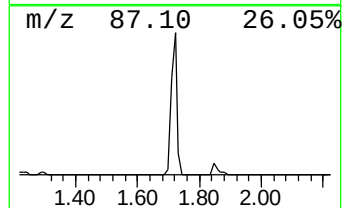
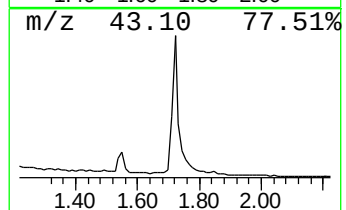
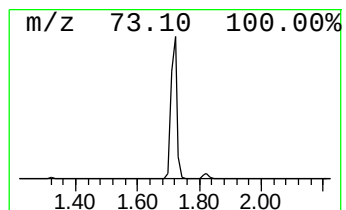
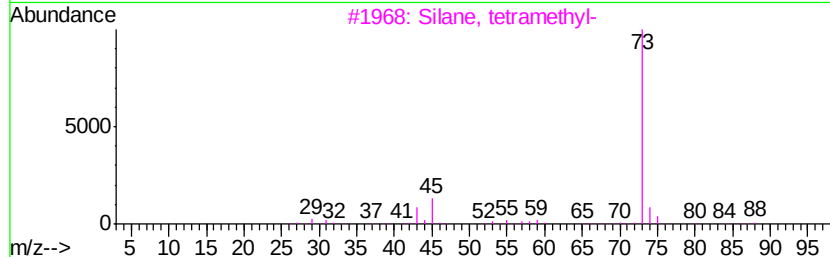
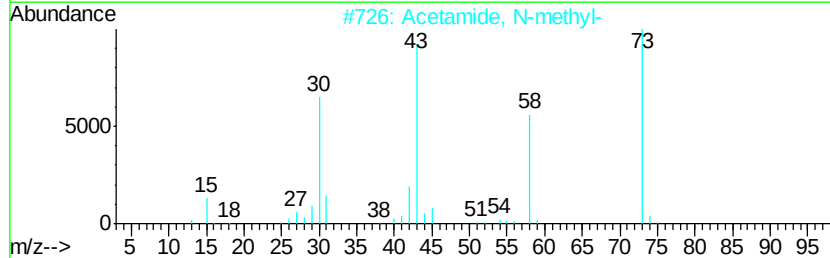
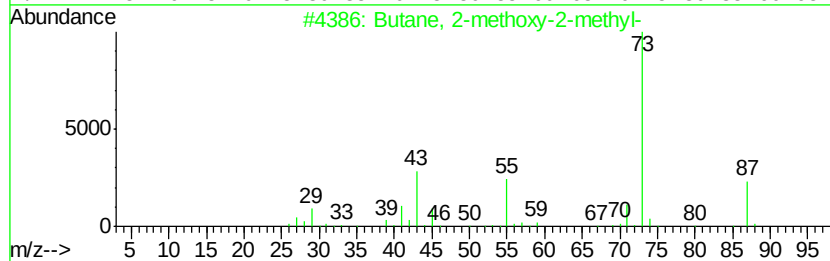
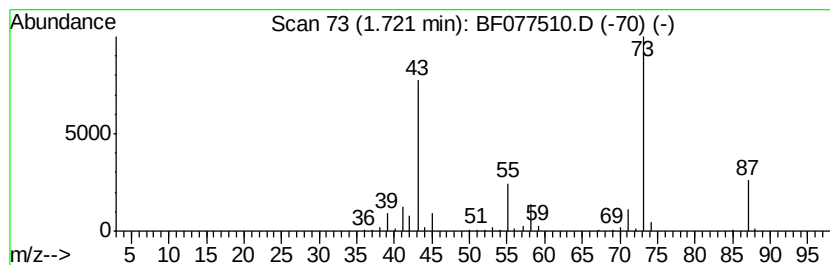
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.72	18.17 ng	373988	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	59
2		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	32
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	10
5		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	10



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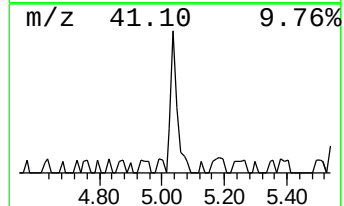
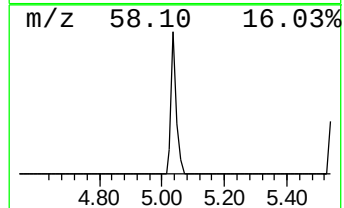
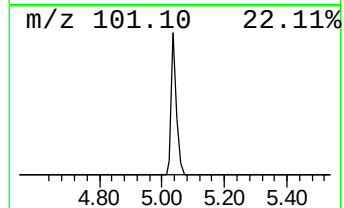
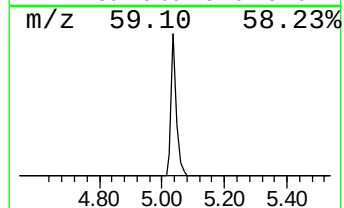
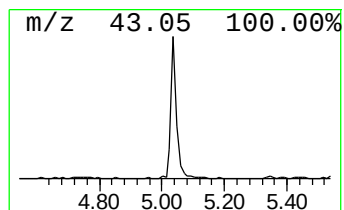
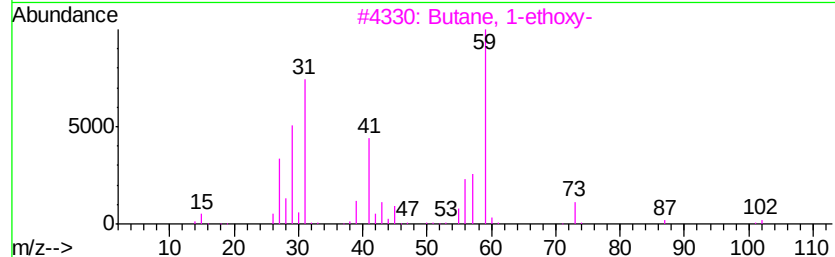
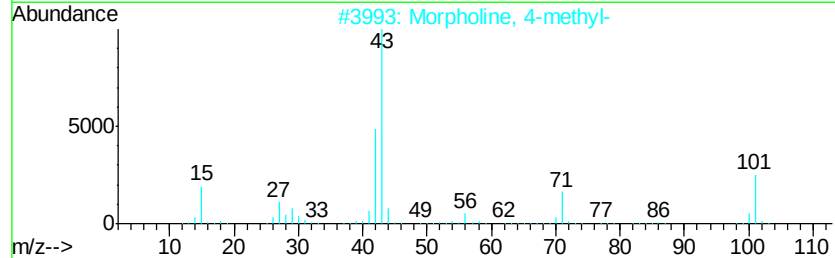
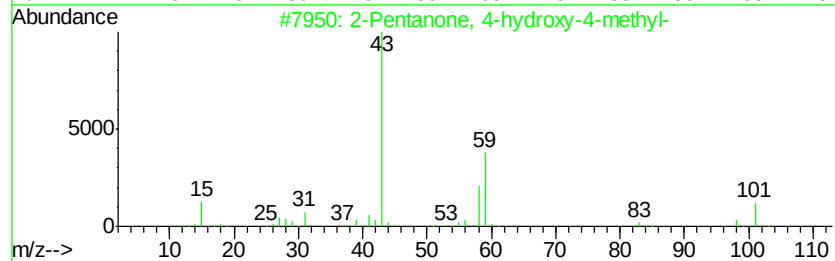
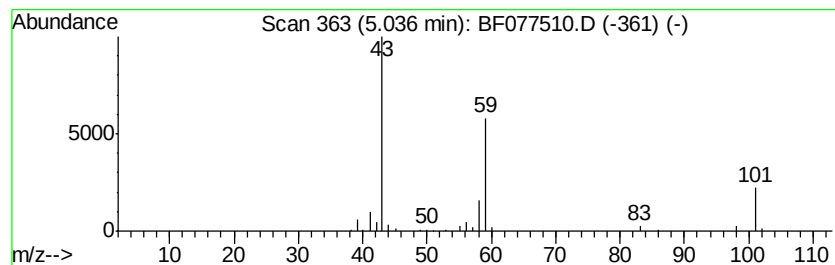
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.04	5.56 ng	114463	1,4-Dichlorobenzene-d4	7.26

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
4		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5		5-Hexen-2-one	98	C6H10O	000109-49-9	9



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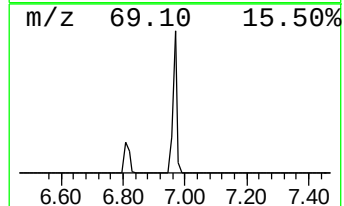
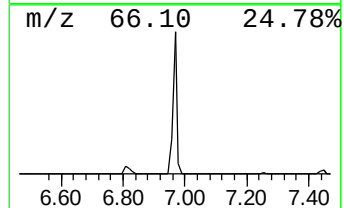
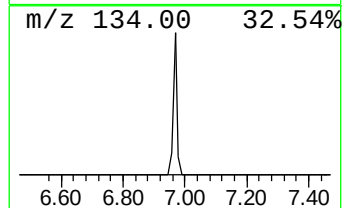
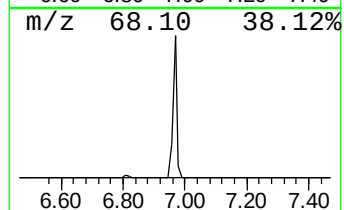
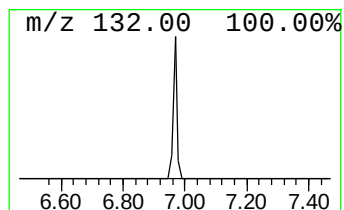
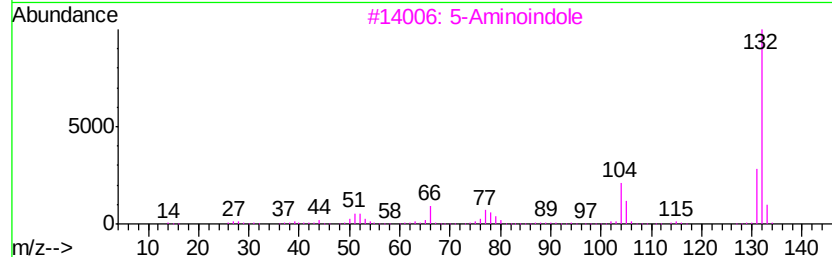
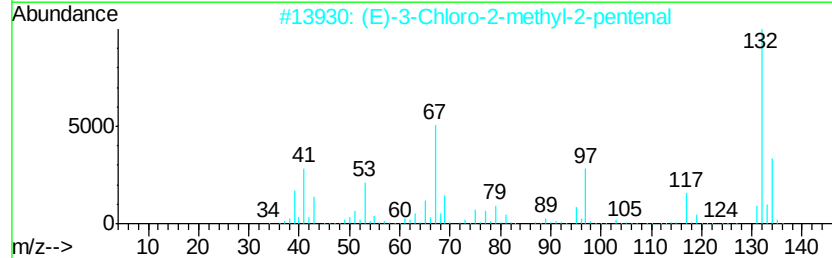
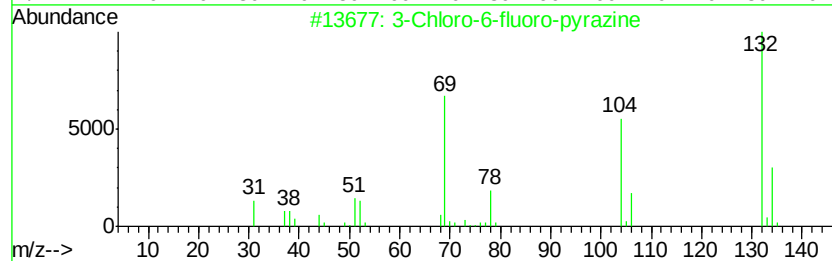
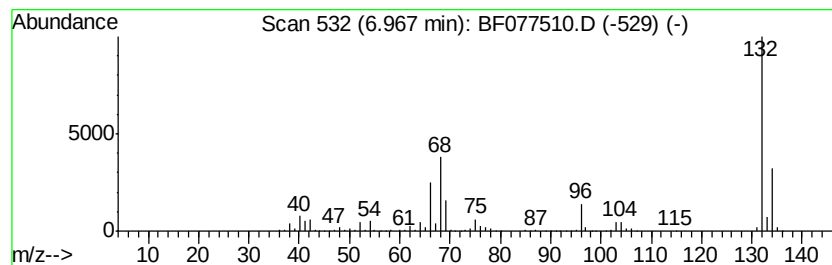
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Peak Number 5 unknown6.97 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.97	63.98 ng	1316720	1,4-Dichlorobenzene-d4	7.26

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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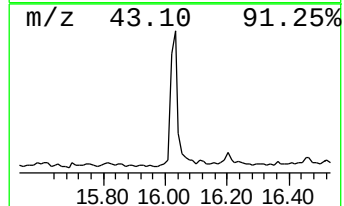
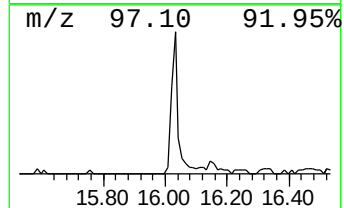
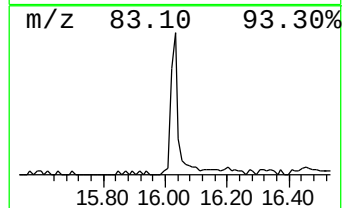
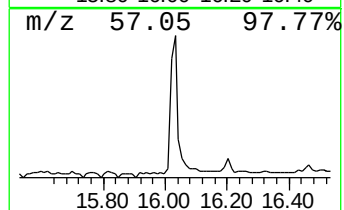
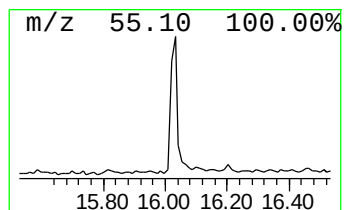
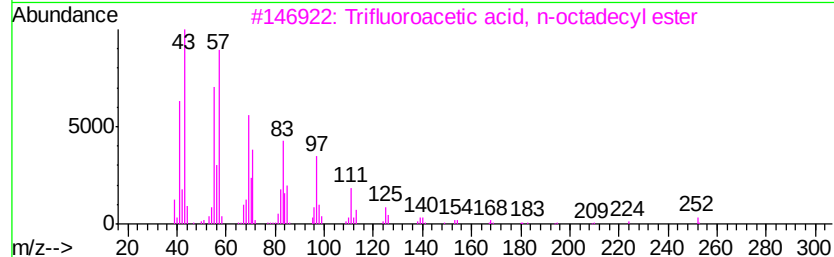
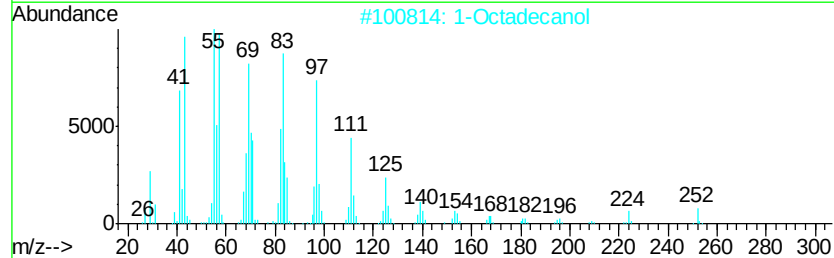
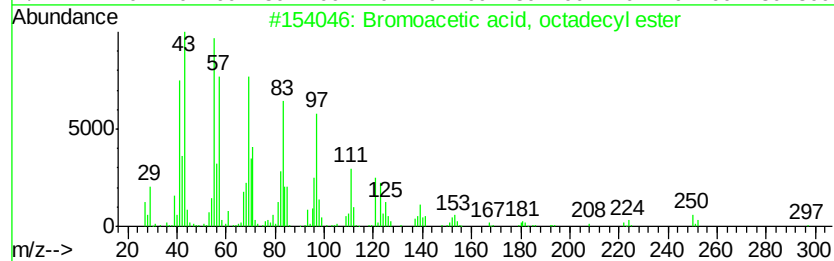
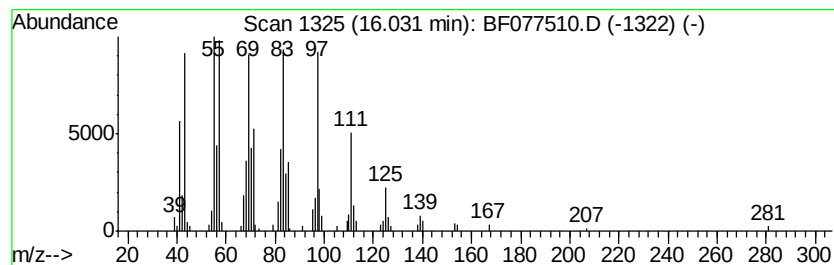
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Peak Number 7 Bromoacetic acid, octadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.03	5.79 ng	246864	Chrysene-d12	16.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		1-Octadecanol	270	C18H38O	000112-92-5	91
3		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		3-Eicosene, (E)-	280	C20H40	074685-33-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	1.72	18.2	ng	373988	1	7.26	411603	20.0
2-Pentanone, 4-hy...	5.04	5.6	ng	114463	1	7.26	411603	20.0
unknown6.97	6.97	64.0	ng	1316720	1	7.26	411603	20.0
Bromoacetic acid,...	16.03	5.8	ng	246864	5	16.15	853041	20.0