

Data Path : Z:\HPCHEM1\BNA F\Data\BF042017\
 Data File : BF094545.D
 Acq On : 20 Apr 2017 15:27
 Operator : SJ/MA
 Sample : I2744-08
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-7(18-20)20170418

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:\HPCHEM1\BNA_F\METHODS\8270-BF041717.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	3.360	238	242	251	rBV	414356	450737	14.68%	1.873%
2	3.478	257	262	266	rVB	47055	48016	1.56%	0.200%
3	3.913	331	336	348	rBV	591747	683378	22.26%	2.839%
4	4.313	400	404	421	rVB	1979695	1802859	58.73%	7.491%
5	5.390	582	587	598	rBV	2150004	2168124	70.63%	9.009%
6	5.513	604	608	612	rBV	2298378	2131297	69.43%	8.856%
7	5.760	647	650	658	rBV	772150	667926	21.76%	2.775%
8	5.942	676	681	684	rBV	1916520	1818083	59.23%	7.554%
9	6.413	756	761	764	rBV	1498299	1464071	47.70%	6.083%
10	7.254	900	904	908	rBV	1018980	926521	30.18%	3.850%
11	8.578	1124	1129	1133	rBV	3009921	2935540	95.63%	12.197%
12	9.078	1210	1214	1218	rBV	648649	565151	18.41%	2.348%
13	9.389	1260	1267	1272	rBV2	1086519	1075382	35.03%	4.468%
14	9.989	1366	1369	1373	rVB	55639	48315	1.57%	0.201%
15	10.260	1407	1415	1418	rBV	20587	33314	1.09%	0.138%
16	10.360	1428	1432	1438	rBV	987178	989052	32.22%	4.110%
17	10.572	1465	1468	1470	rBV	64592	63115	2.06%	0.262%
18	11.124	1558	1562	1565	rBV	36928	34053	1.11%	0.141%
19	11.207	1572	1576	1580	rBV	1054779	1076788	35.08%	4.474%
20	13.189	1908	1913	1917	rBV	2601491	3069644	100.00%	12.754%
21	14.354	2107	2111	2123	rBV2	105618	190014	6.19%	0.790%
22	14.454	2123	2128	2132	rVV	897827	959070	31.24%	3.985%
23	14.513	2132	2138	2143	rVB	30872	56373	1.84%	0.234%
24	15.571	2314	2318	2323	rVB	45290	45683	1.49%	0.190%
25	16.077	2400	2404	2416	rBV	671123	764867	24.92%	3.178%

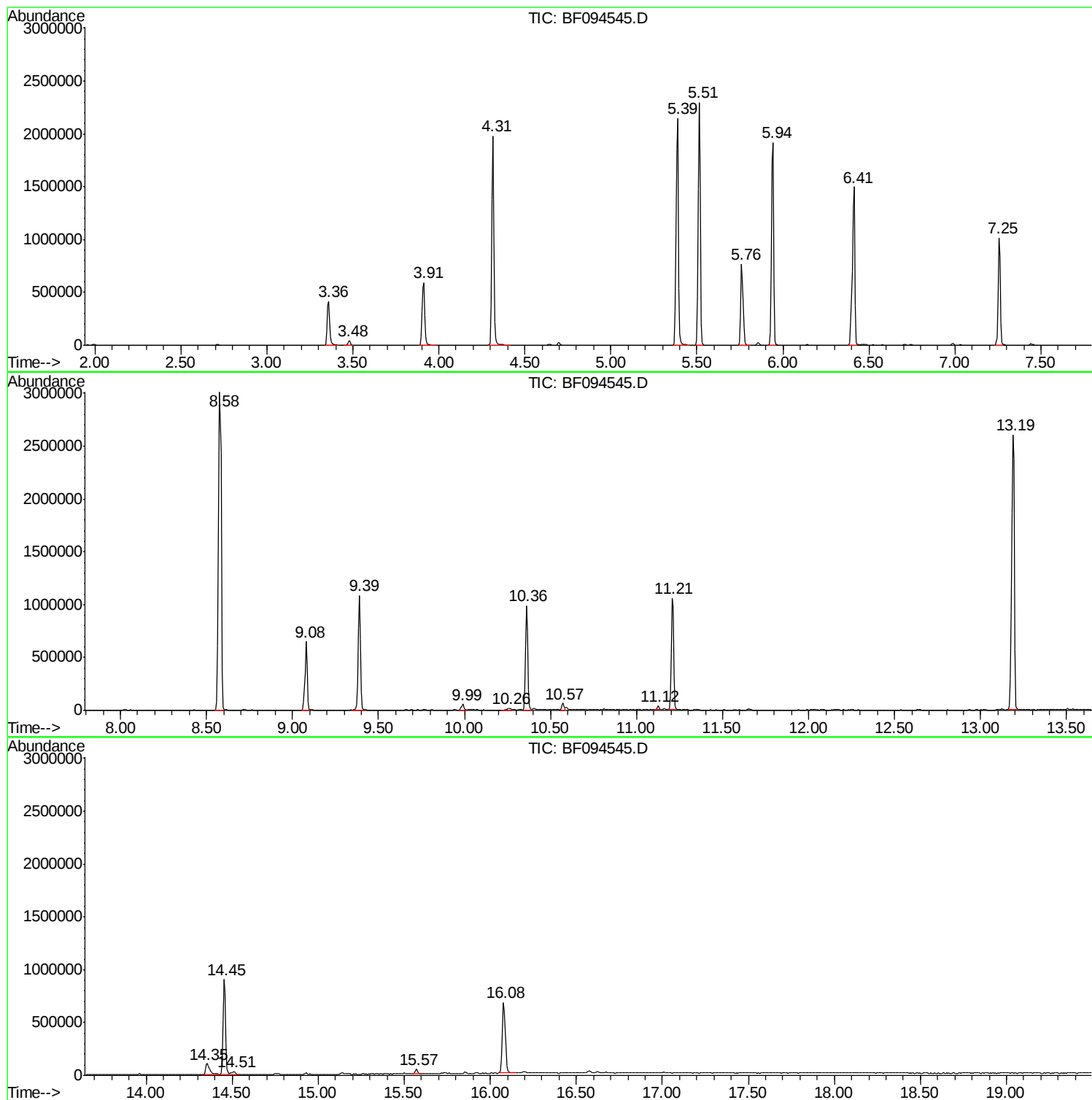
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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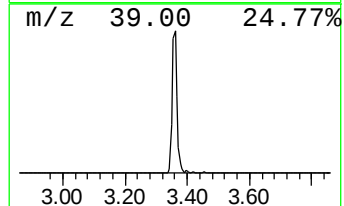
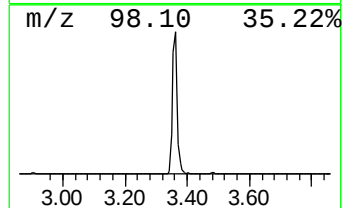
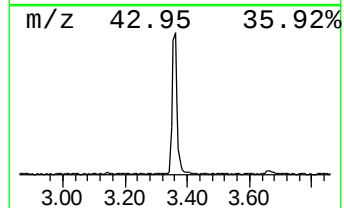
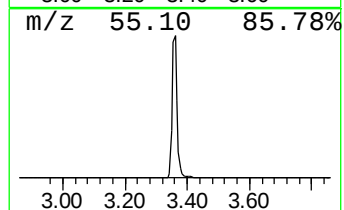
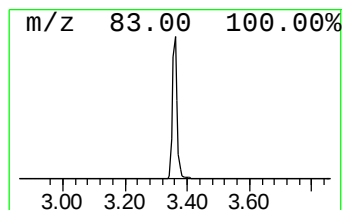
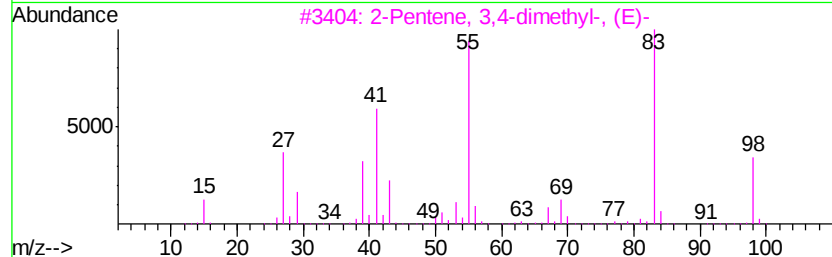
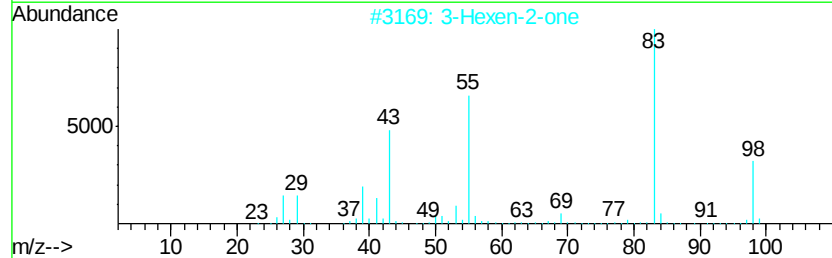
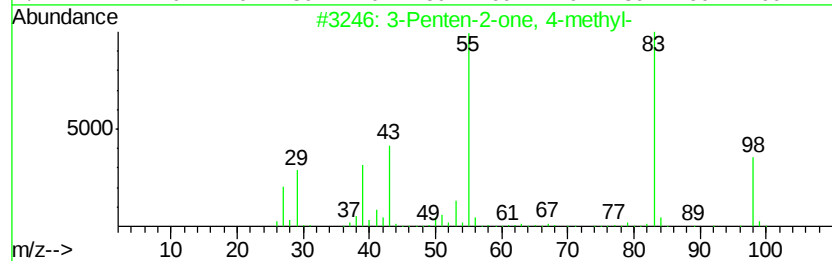
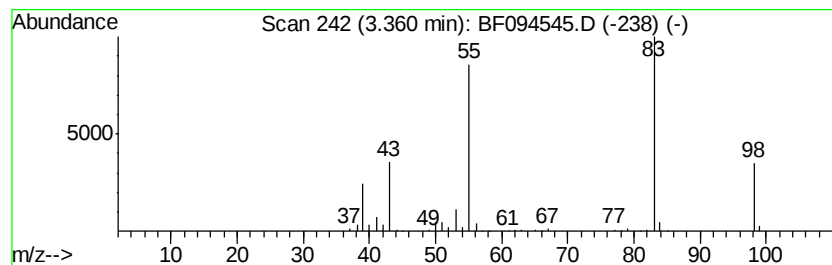
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF041717.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.36	13.50 ng	450737	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	94
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	80



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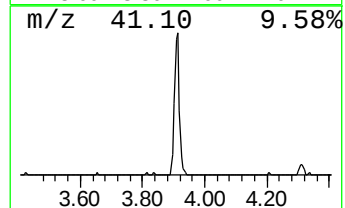
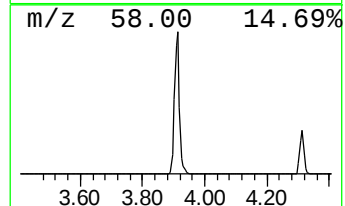
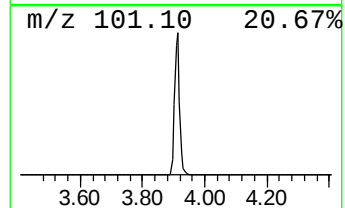
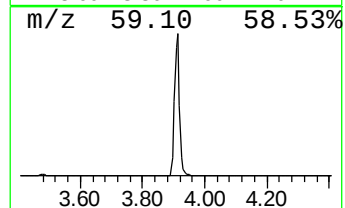
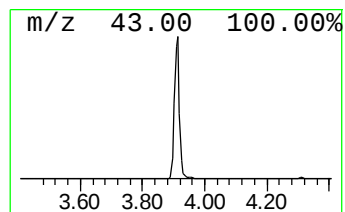
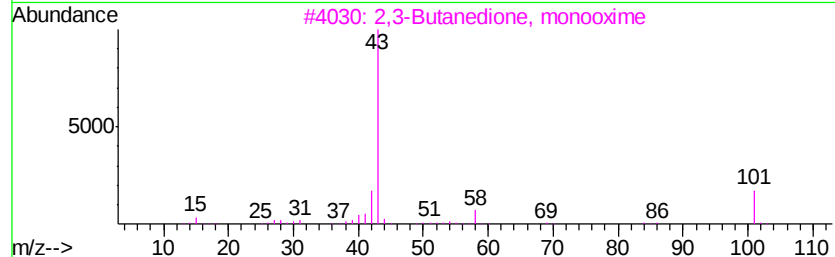
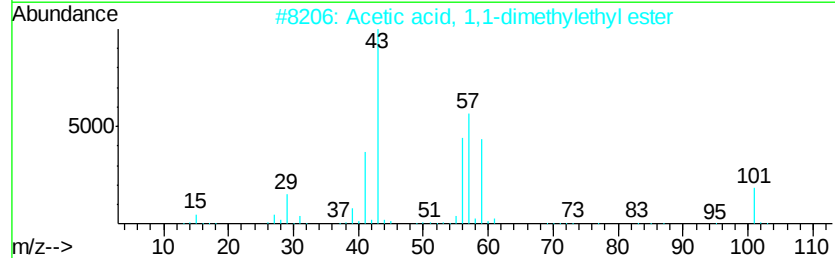
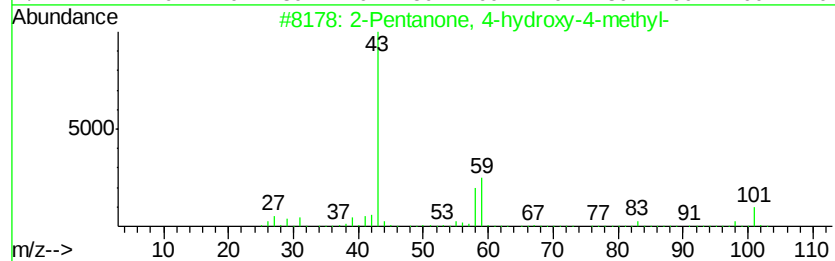
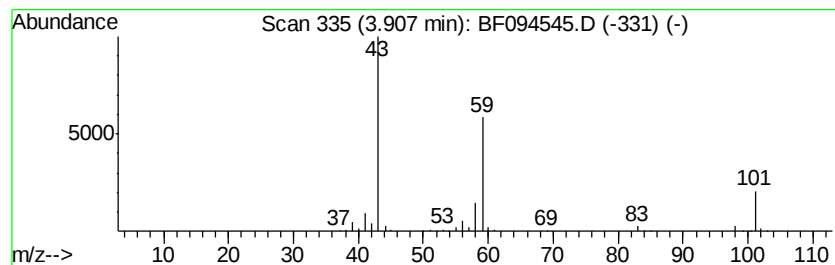
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	20.46 ng	683378	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	38
4		3-Hexanol	102	C6H14O	000623-37-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17



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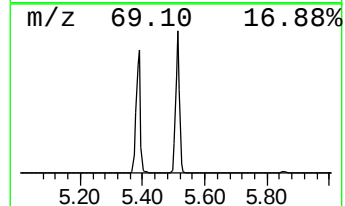
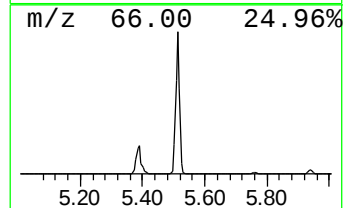
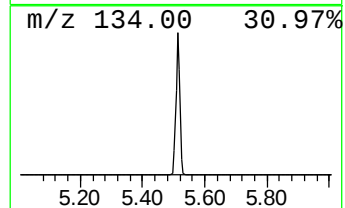
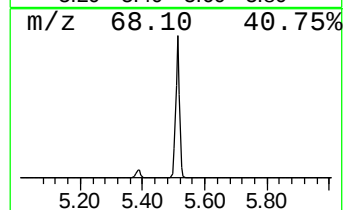
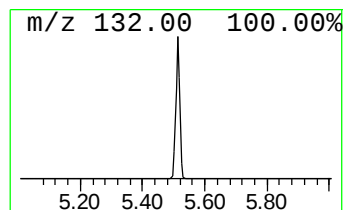
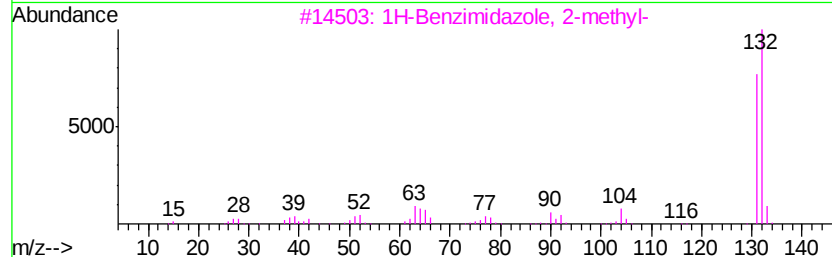
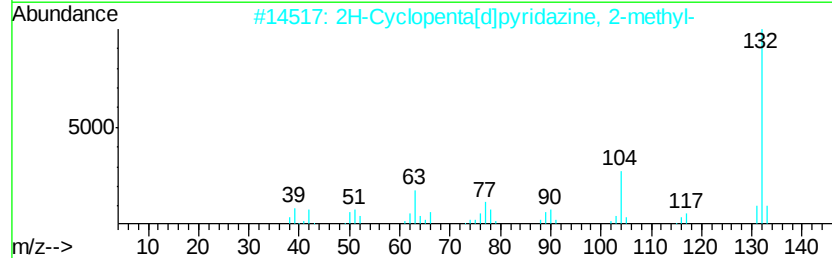
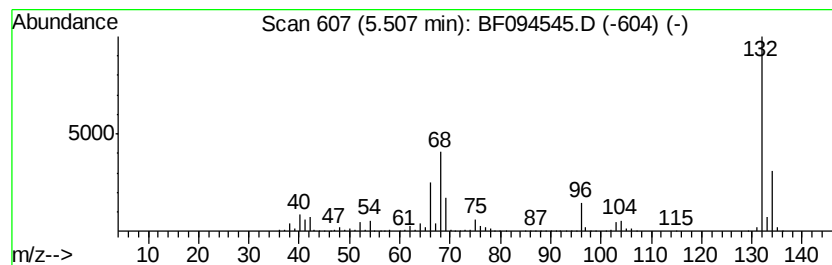
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Peak Number 3 unknown5.51 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.51	63.82 ng	2131300	1,4-Dichlorobenzene-d4	5.76

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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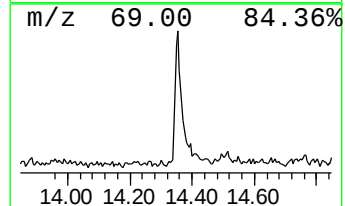
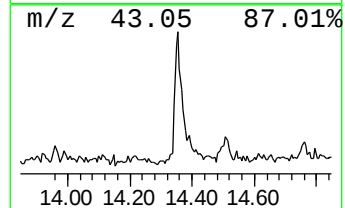
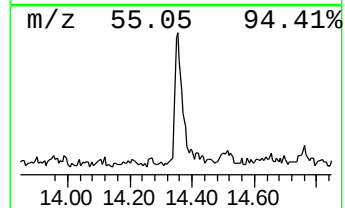
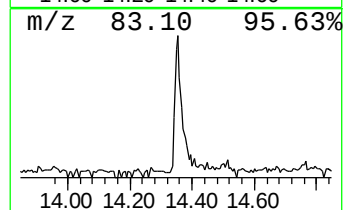
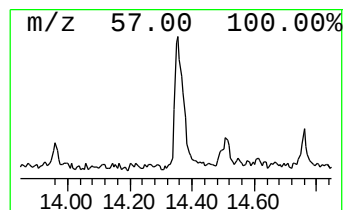
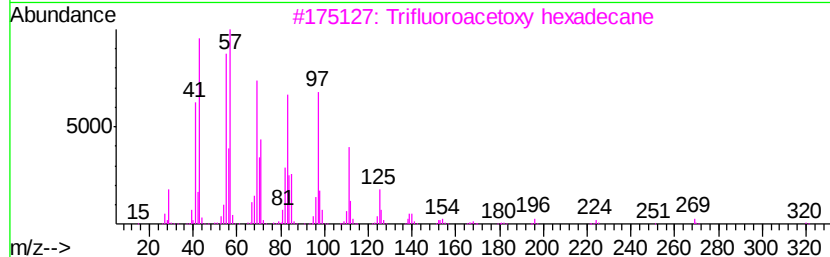
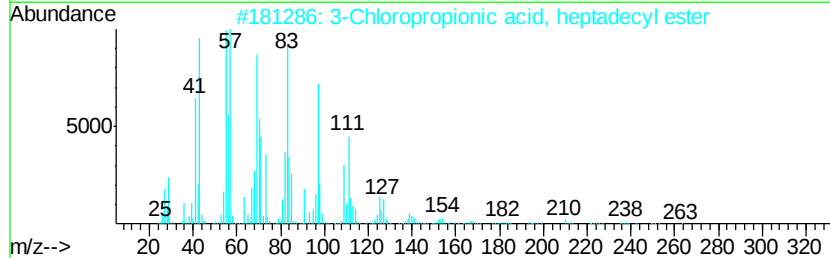
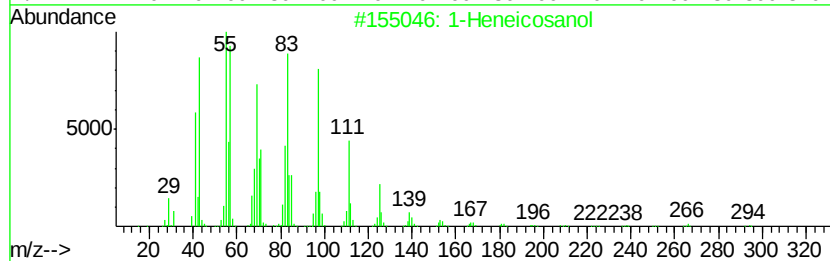
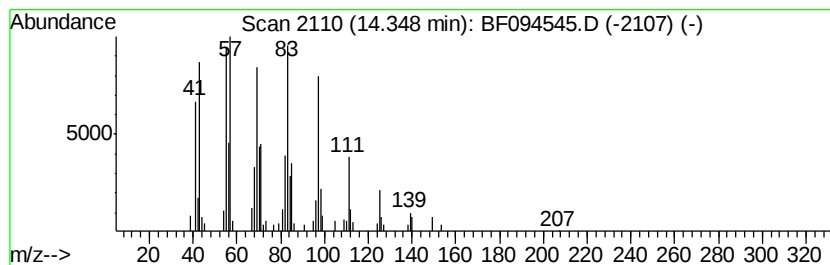
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.35	3.96 ng	190014	Chrysene-d12	14.45
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heneicosanol	312 C21H44O	015594-90-8 93
2		3-Chloropropionic acid, heptadec...	346 C20H39ClO2	1000283-05-1 90
3		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 87
4		n-Heptadecanol-1	256 C17H36O	001454-85-9 87
5		Trichloroacetic acid, pentadecyl...	372 C17H31Cl3O2	074339-53-0 81



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one, 4...	3.36	13.5	ng	450737	1	5.76	667926	20.0
2-Pentanone, 4-hy...	3.91	20.5	ng	683378	1	5.76	667926	20.0
unknown5.51	5.51	63.8	ng	2131300	1	5.76	667926	20.0
1-Heneicosanol	14.35	4.0	ng	190014	5	14.45	959070	20.0