

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF040418\
 Data File : BF104245.D
 Acq On : 5 Apr 2018 00:05
 Operator : JU/SJ
 Sample : J2203-01
 Misc :
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 FK-BPM-01-D02-D02A-E02-E02A

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-BF032818.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	2.275	27	32	41	rVB	89102	129329	4.63%	0.588%
2	5.187	524	527	535	rBV	59200	102108	3.65%	0.464%
3	5.587	592	595	627	rBV	733793	1942334	69.48%	8.832%
4	6.592	762	766	785	rBV	930927	2105424	75.32%	9.574%
5	6.722	785	788	824	rVV	1524886	2795399	100.00%	12.711%
6	6.951	824	827	849	rVV	276778	731318	26.16%	3.326%
7	7.104	849	853	885	rVB	1335330	1935962	69.26%	8.803%
8	7.516	920	923	946	rBV	628513	1351502	48.35%	6.146%
9	8.234	1041	1045	1070	rBV	499651	916532	32.79%	4.168%
10	9.304	1223	1227	1243	rBV	1988331	2694156	96.38%	12.251%
11	9.698	1287	1294	1299	rBV	128835	179144	6.41%	0.815%
12	9.892	1323	1327	1330	rBV	61041	50527	1.81%	0.230%
13	9.986	1339	1343	1362	rBV	879127	1018647	36.44%	4.632%
14	10.392	1409	1412	1415	rBV	78298	55380	1.98%	0.252%
15	10.786	1475	1479	1490	rBV	967486	1399564	50.07%	6.364%
16	10.863	1490	1492	1506	rVB	78394	125546	4.49%	0.571%
17	11.486	1594	1598	1619	rBV	599351	904096	32.34%	4.111%
18	12.863	1829	1832	1836	rBV	51332	48345	1.73%	0.220%
19	13.063	1863	1866	1887	rBV	1735504	2055085	73.52%	9.345%
20	13.568	1949	1952	1955	rVB	40002	32147	1.15%	0.146%
21	13.939	2011	2015	2020	rBV	61179	66663	2.38%	0.303%
22	14.139	2045	2049	2066	rBV	477468	681370	24.37%	3.098%
23	14.962	2186	2189	2194	rVB	85659	86918	3.11%	0.395%
24	15.674	2305	2310	2325	rVV	304043	554511	19.84%	2.522%
25	16.086	2377	2380	2384	rVB4	22070	29186	1.04%	0.133%

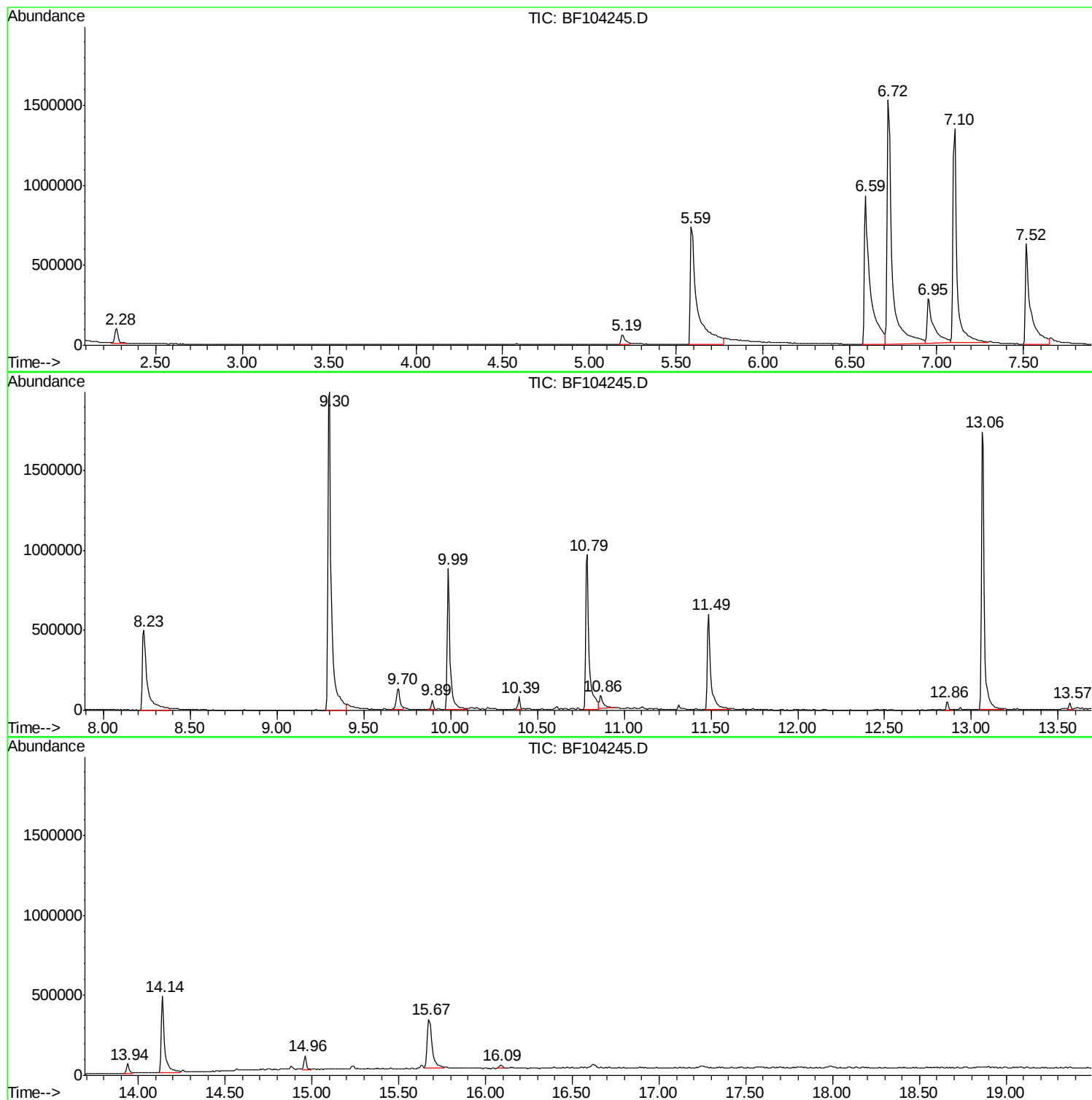
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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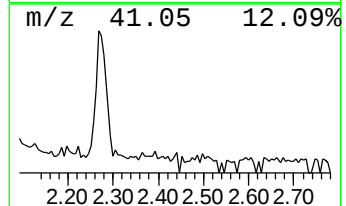
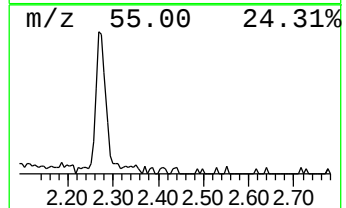
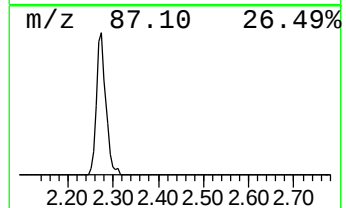
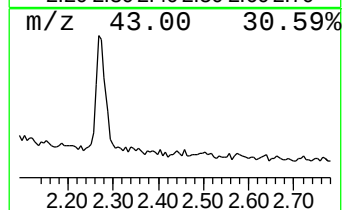
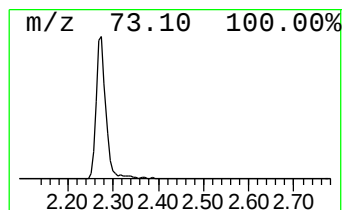
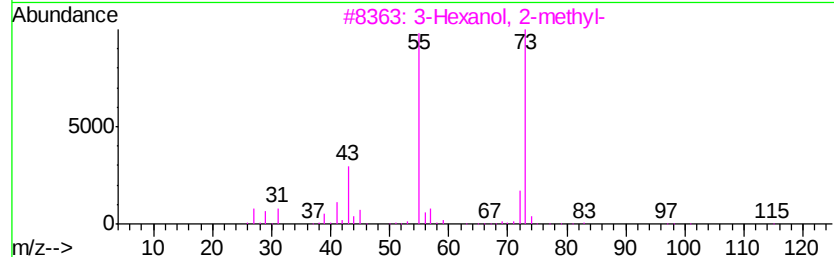
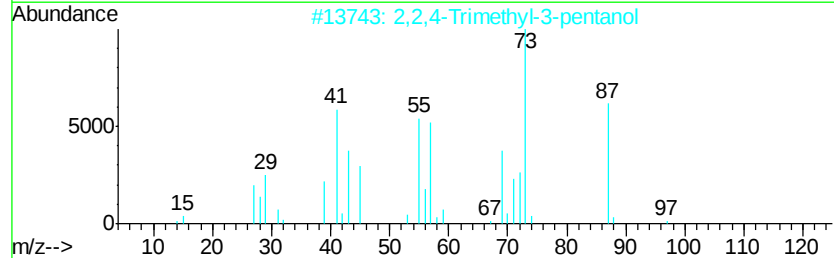
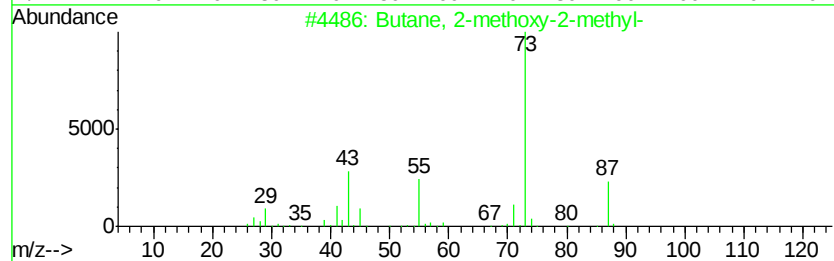
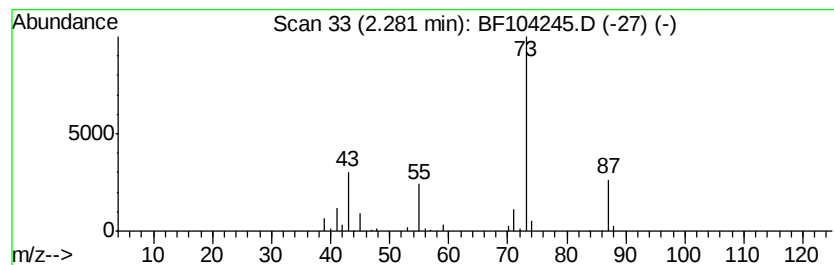
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF032818.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.28	3.54 ng	129329	1,4-Dichlorobenzene-d4	6.95

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	64
3			3-Hexanol, 2-methyl-	116	C7H16O	000617-29-8	17
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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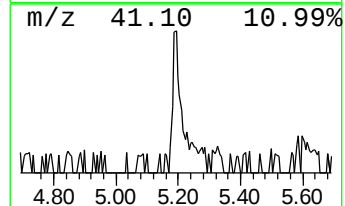
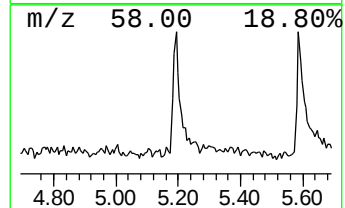
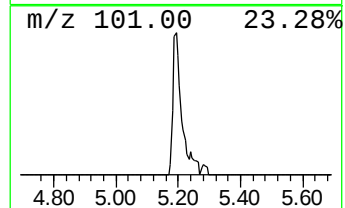
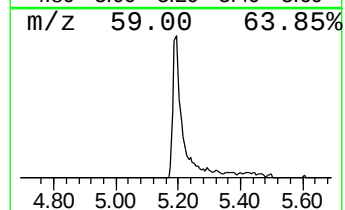
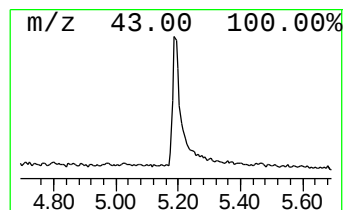
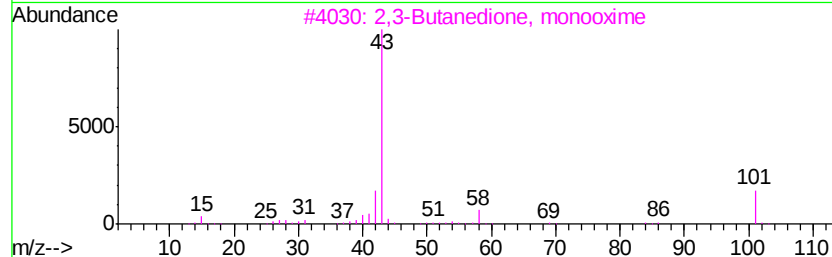
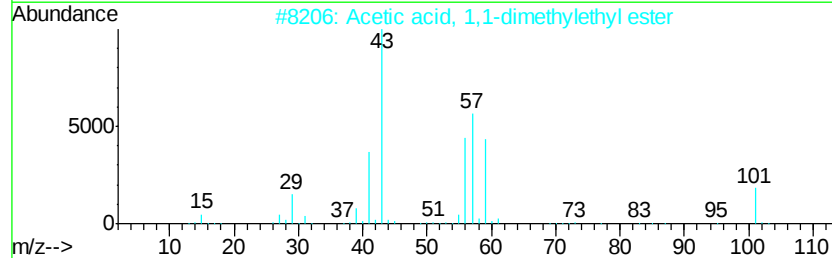
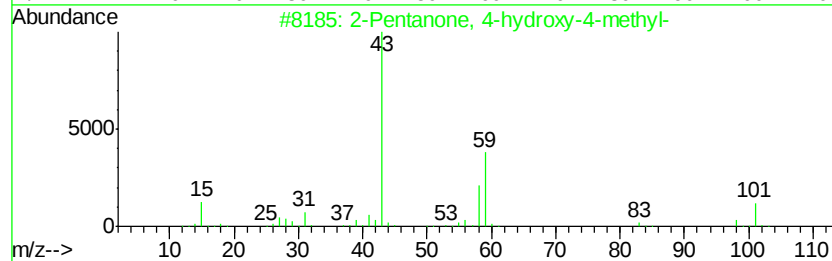
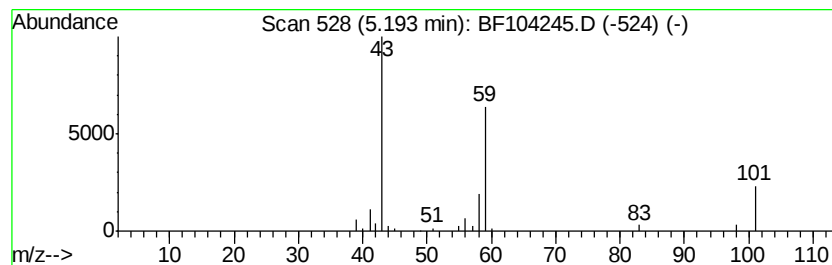
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.79 ng	102108	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	25
5		5-Hexen-2-one	98	C6H10O	000109-49-9	10



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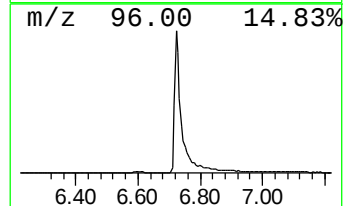
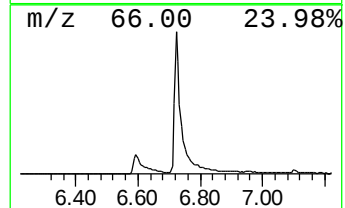
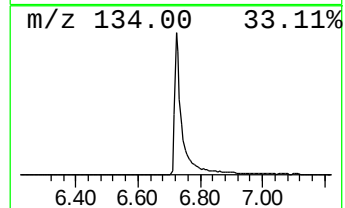
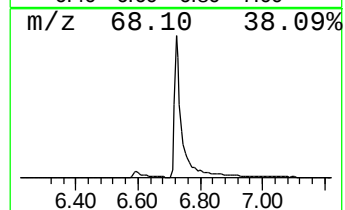
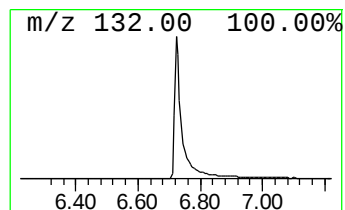
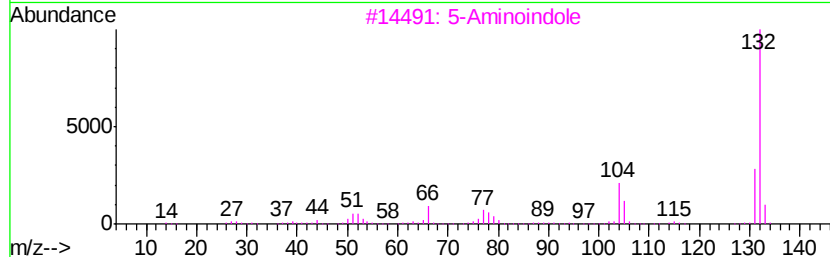
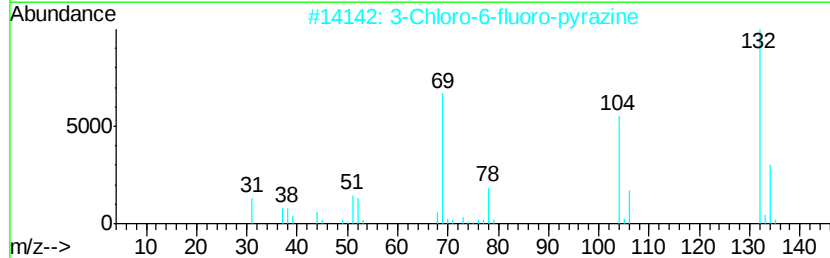
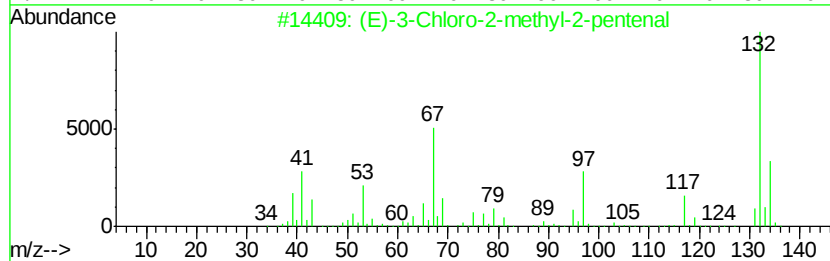
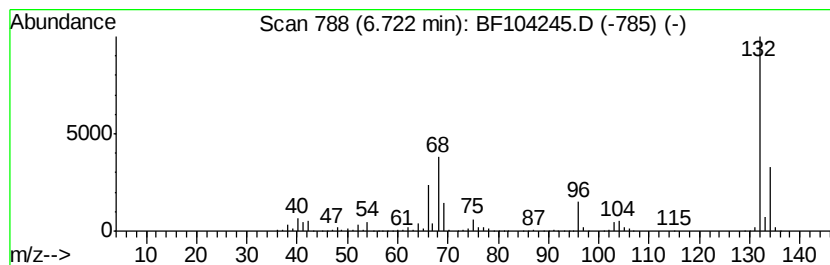
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Peak Number 3 unknown6.72 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.72	76.45 ng	2795400	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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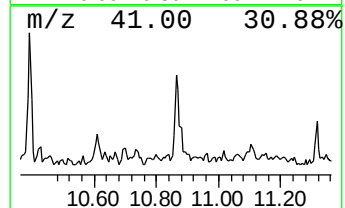
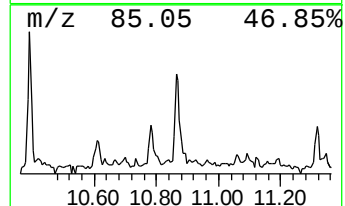
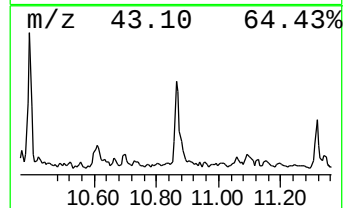
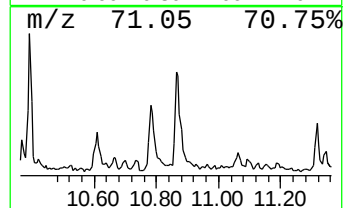
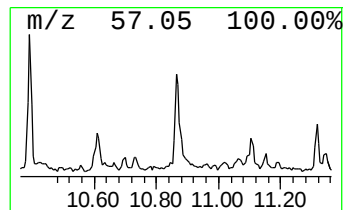
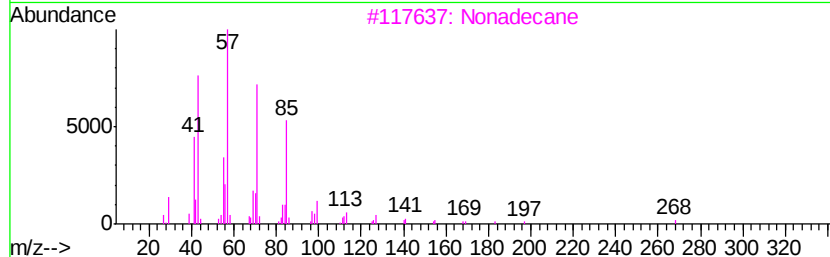
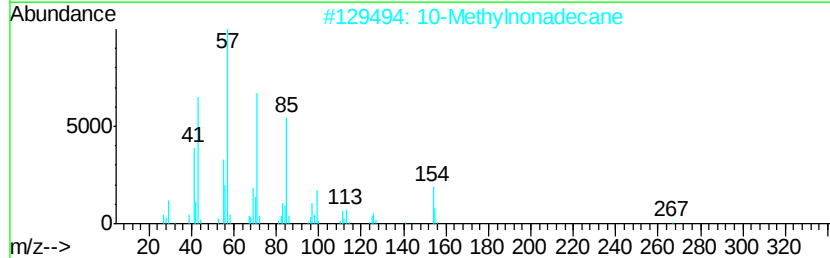
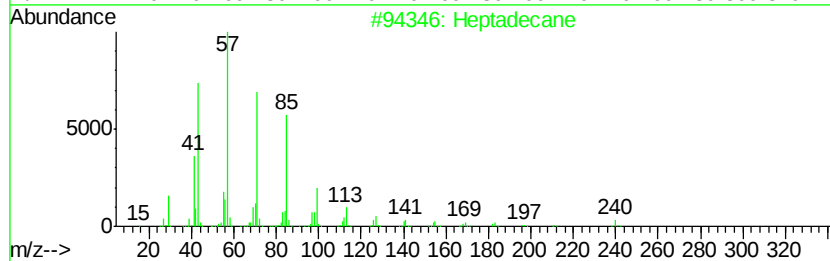
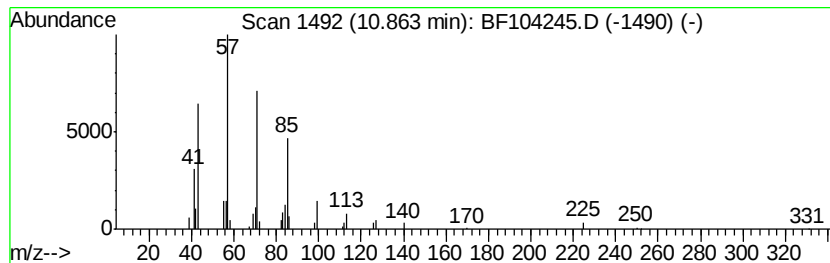
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Peak Number 5 Heptadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.86	2.78 ng	125546	Phenanthrene-d10	11.49
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Heptadecane	240 C17H36	000629-78-7	90
2	10-Methylnonadecane	282 C20H42	056862-62-5	86
3	Nonadecane	268 C19H40	000629-92-5	86
4	Tetradecane	198 C14H30	000629-59-4	86
5	Hexadecane	226 C16H34	000544-76-3	83



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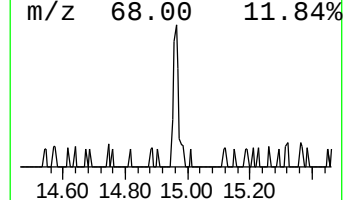
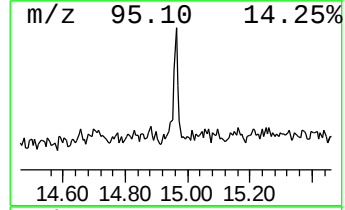
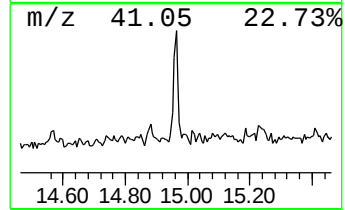
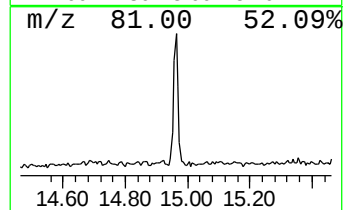
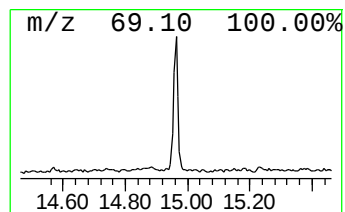
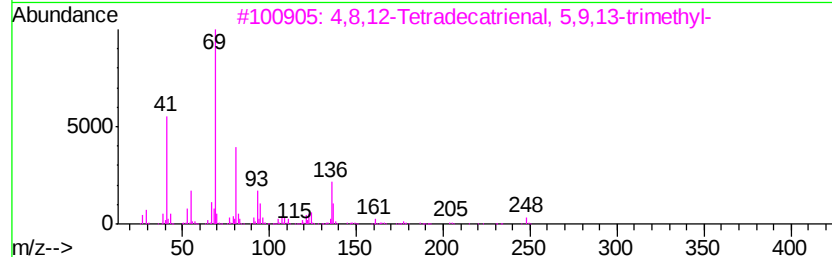
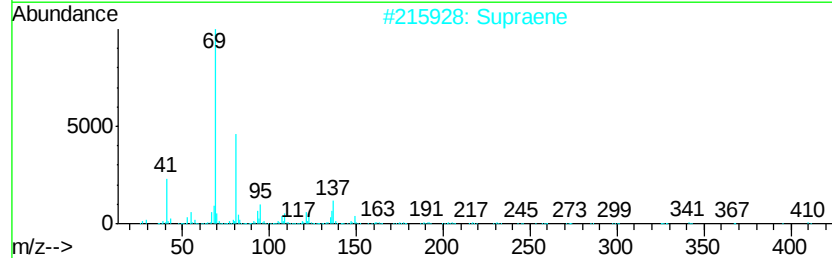
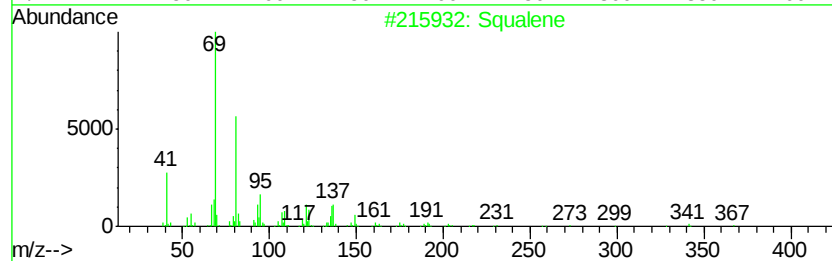
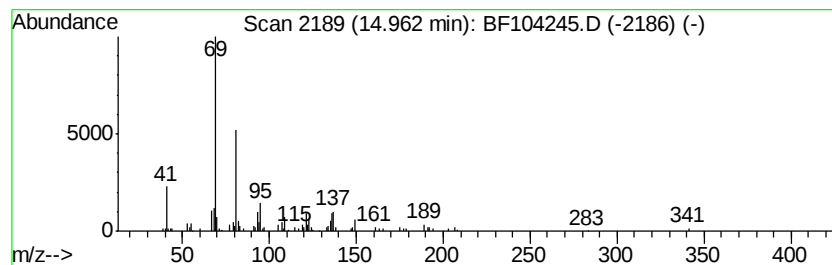
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Peak Number 6 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.96	3.13 ng	86918	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		trans-Farnesol	222	C15H26O	000106-28-5	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.28	3.5	ng	129329	1	6.95	731318	20.0
2-Pentanone, 4-hy...	5.19	2.8	ng	102108	1	6.95	731318	20.0
unknown6.72	6.72	76.5	ng	2795400	1	6.95	731318	20.0
Heptadecane	10.86	2.8	ng	125546	4	11.49	904096	20.0
Squalene	14.96	3.1	ng	86918	6	15.67	554511	20.0