

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071316\
 Data File : BG023075.D
 Acq On : 13 Jul 2016 18:30
 Operator : UM/SJ
 Sample : H3946-15
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 P7-B5(6-12)C

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:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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	3.040	29	34	52	rBV	6175251	9425708	100.00%	16.039%
2	5.225	399	406	413	rBV	425302	635943	6.75%	1.082%
3	5.701	480	487	497	rBV	1878288	3038703	32.24%	5.171%
4	7.311	753	761	770	rBV	2164408	3739748	39.68%	6.364%
5	7.681	817	824	833	rBV	1963233	3417477	36.26%	5.815%
6	8.151	897	904	912	rBV	390758	669109	7.10%	1.139%
7	8.480	951	960	967	rBV	1321455	2320479	24.62%	3.949%
8	9.327	1096	1104	1113	rBV	1295745	2369910	25.14%	4.033%
9	10.983	1378	1386	1394	rBV	591537	1078701	11.44%	1.836%
10	13.416	1791	1800	1810	rBV	3556124	5910307	62.70%	10.057%
11	14.238	1933	1940	1947	rBV	868407	1278604	13.57%	2.176%
12	14.802	2028	2036	2048	rBV2	1126254	1898456	20.14%	3.230%
13	16.295	2283	2290	2302	rBV	3912247	5960710	63.24%	10.143%
14	16.483	2318	2322	2331	rBV2	68765	135928	1.44%	0.231%
15	17.282	2454	2458	2463	rBV	132035	167552	1.78%	0.285%
16	17.558	2498	2505	2514	rBV	1579895	2484982	26.36%	4.228%
17	18.428	2648	2653	2663	rBV	349255	521456	5.53%	0.887%
18	19.691	2865	2868	2874	rVB6	78496	104105	1.10%	0.177%
19	20.161	2942	2948	2954	rBV	6239167	8307839	88.14%	14.137%
20	21.471	3167	3171	3181	rBV6	164335	295265	3.13%	0.502%
21	21.871	3231	3239	3248	rBV	1512841	2635323	27.96%	4.484%
22	25.255	3806	3815	3828	rVB2	791398	2372230	25.17%	4.037%

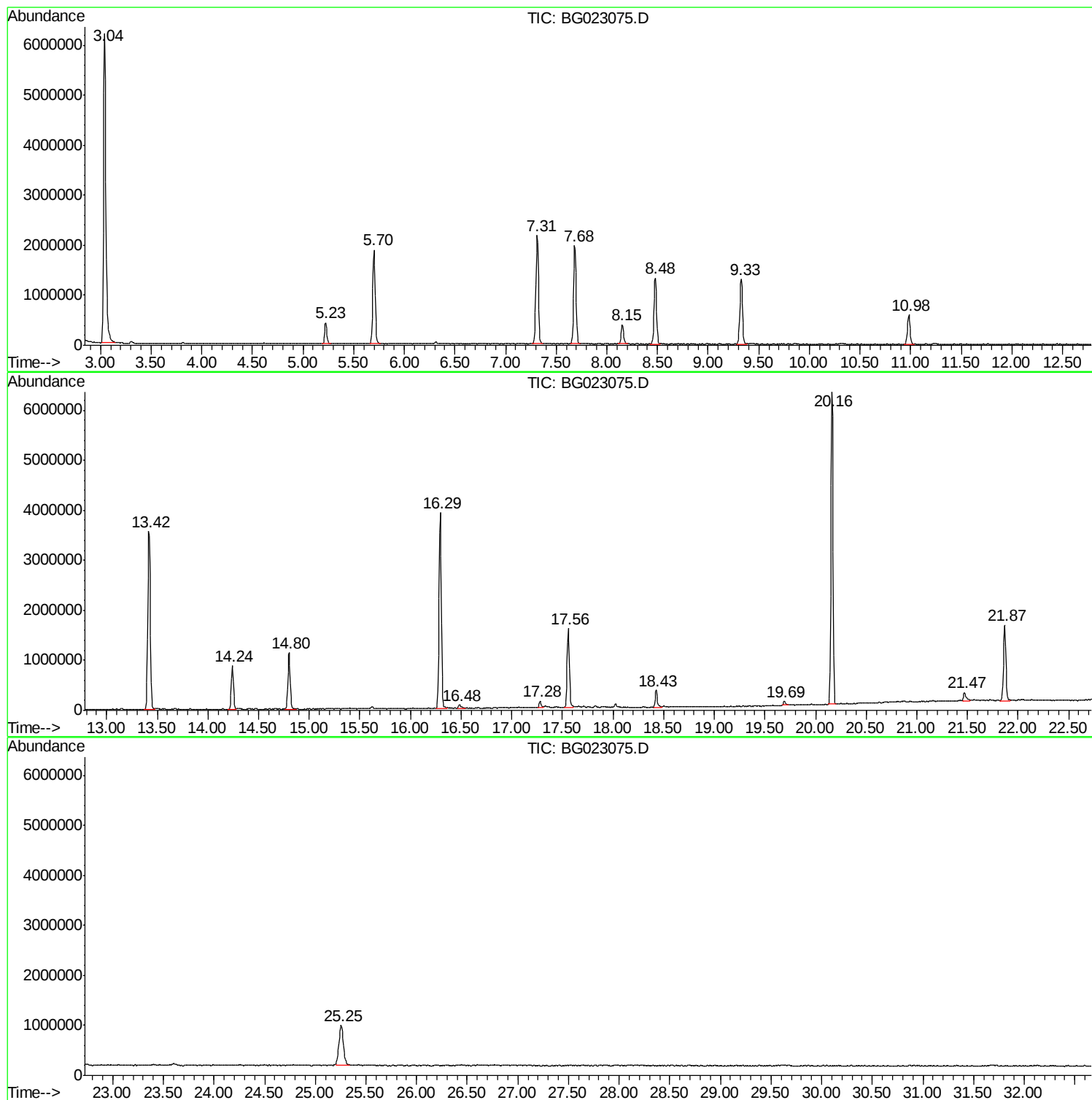
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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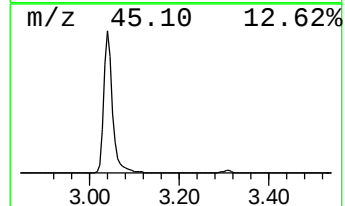
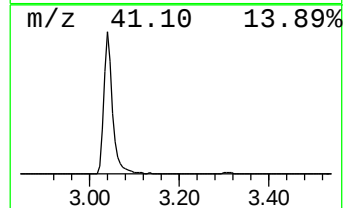
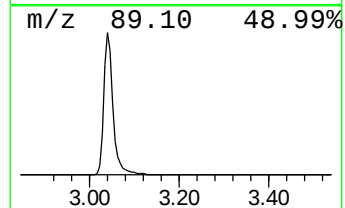
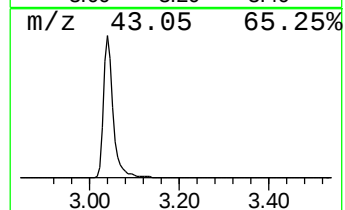
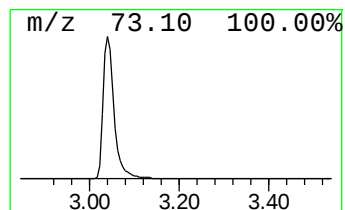
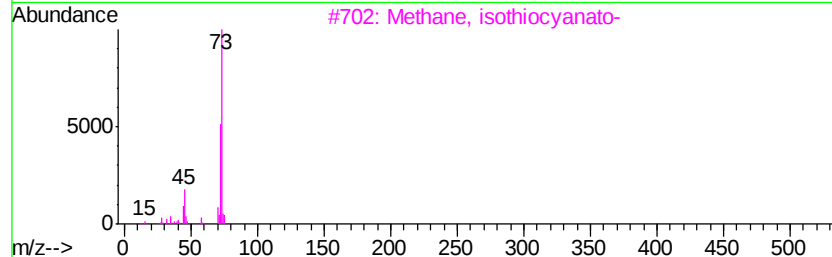
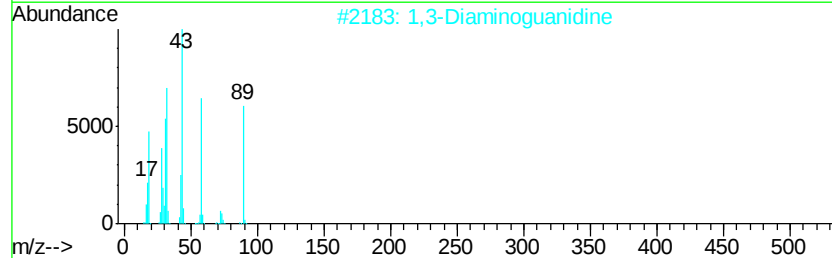
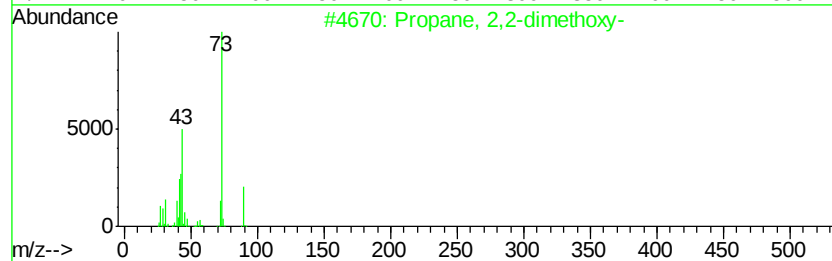
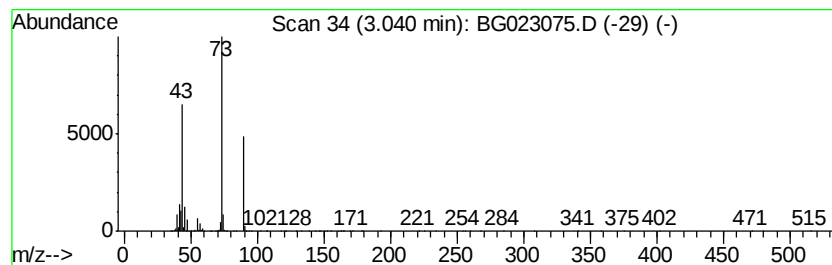
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.04	281.74 ng	9425710	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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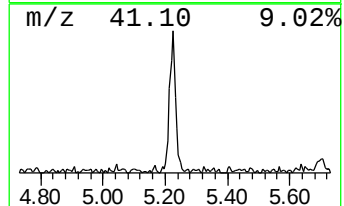
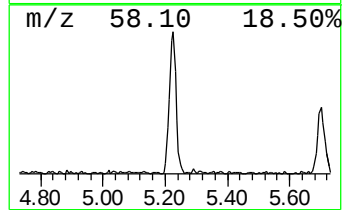
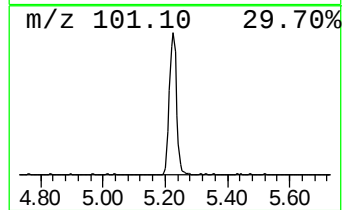
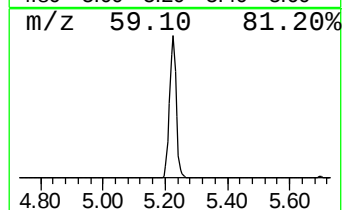
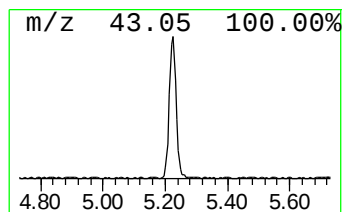
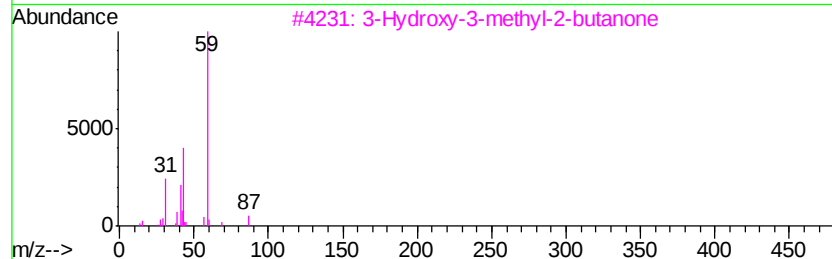
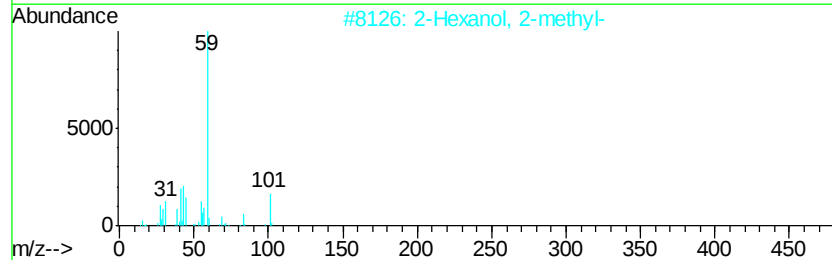
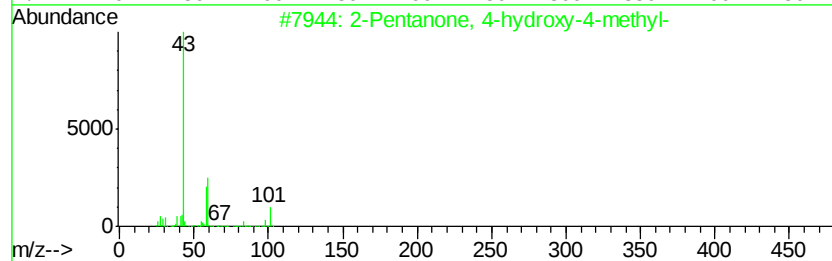
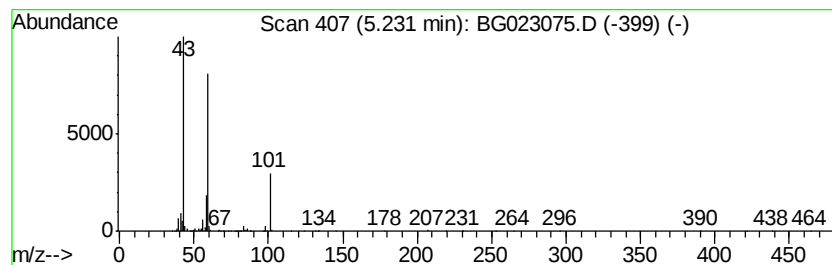
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.23	19.01 ng	635943	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	38
3		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	38
4		Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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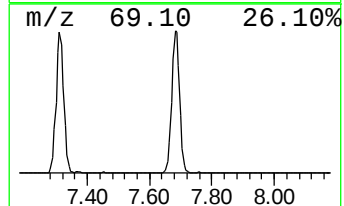
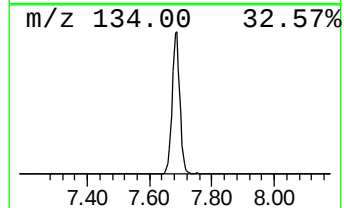
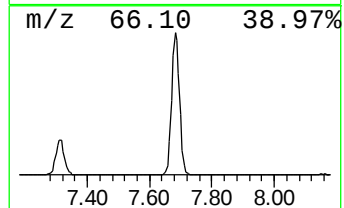
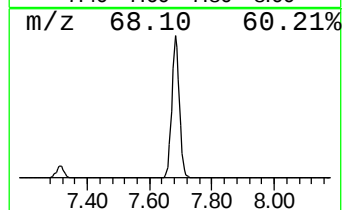
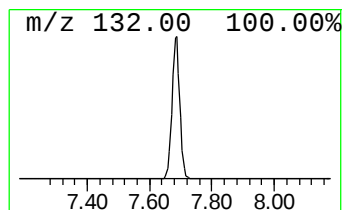
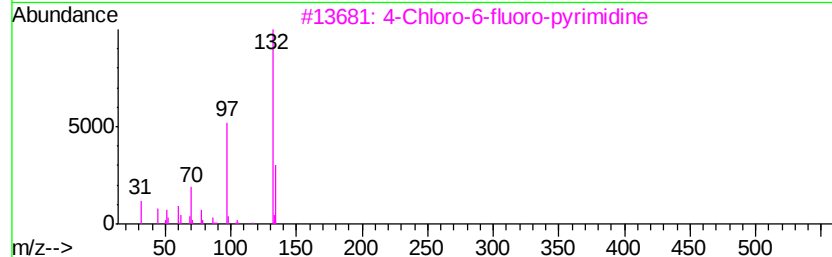
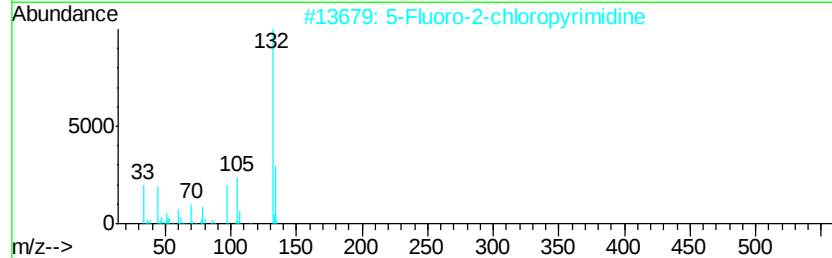
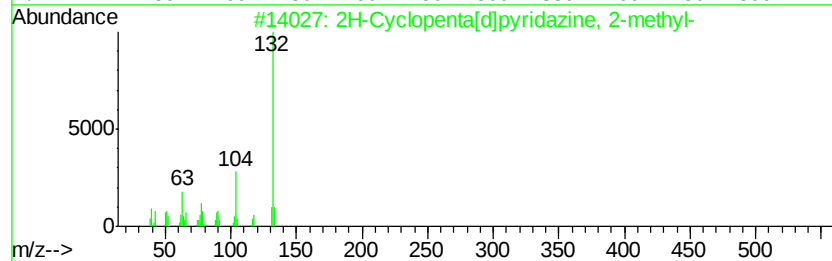
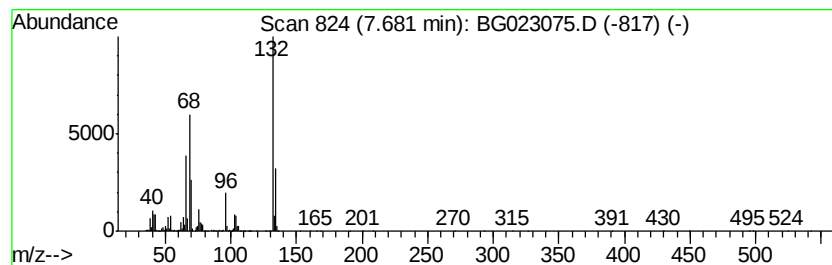
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Peak Number 3 unknown7.68 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	102.15 ng	3417480	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	18
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	14
3		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11



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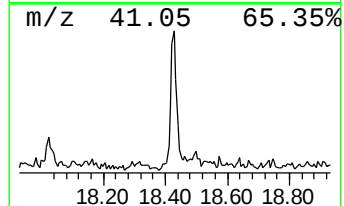
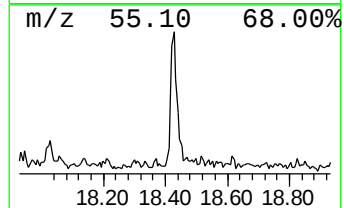
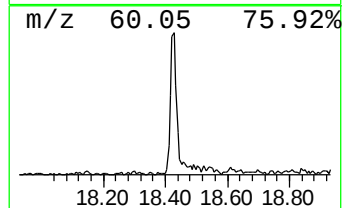
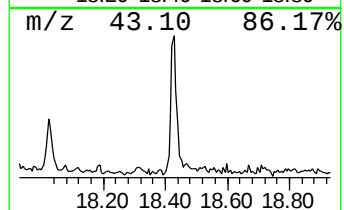
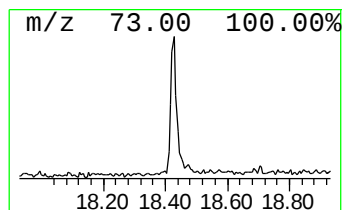
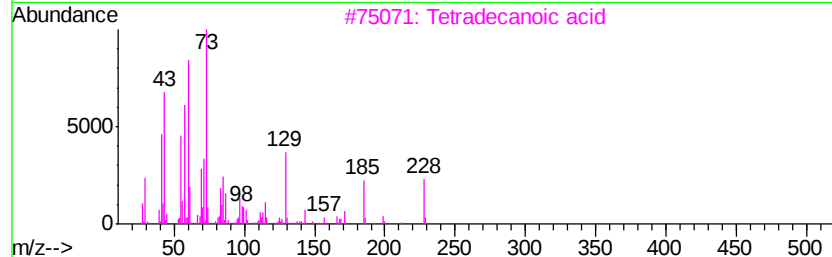
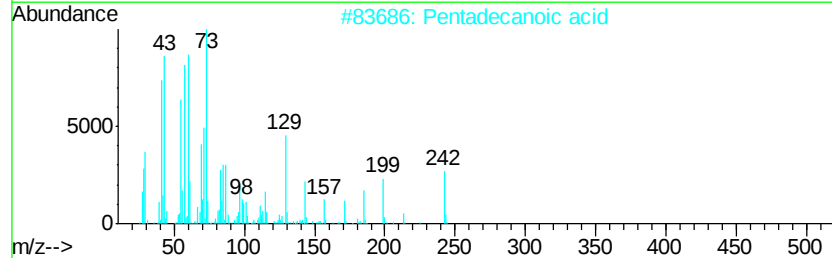
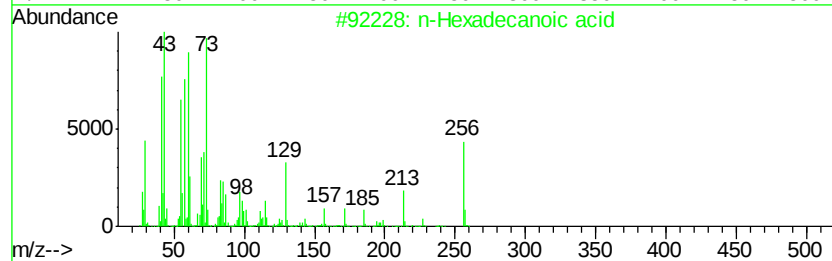
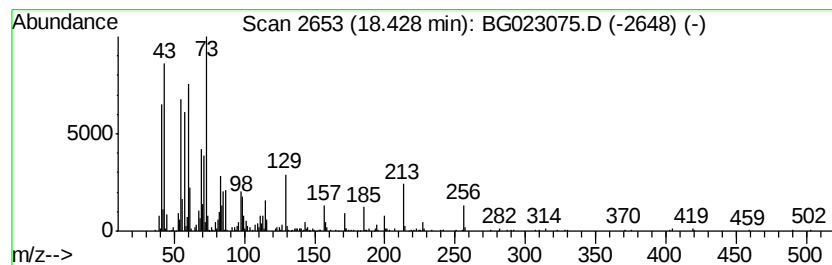
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	4.20 ng	521456	Phenanthrene-d10	17.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		l-(+)-Ascorbic acid 2,6-dihexade...	652	C38H68O8	028474-90-0	45



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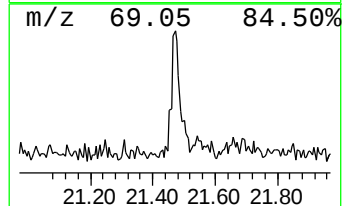
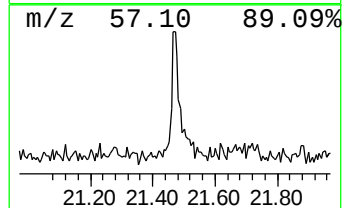
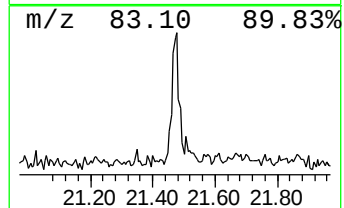
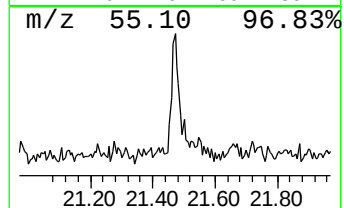
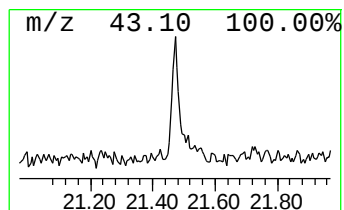
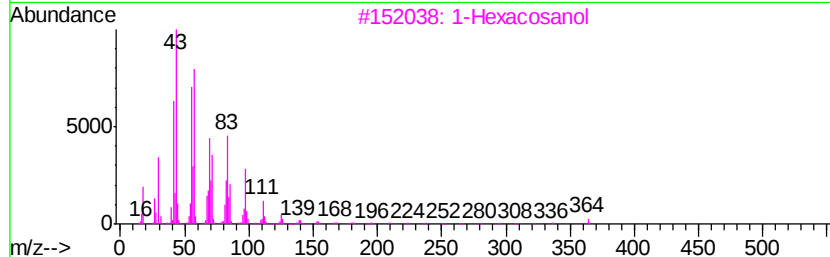
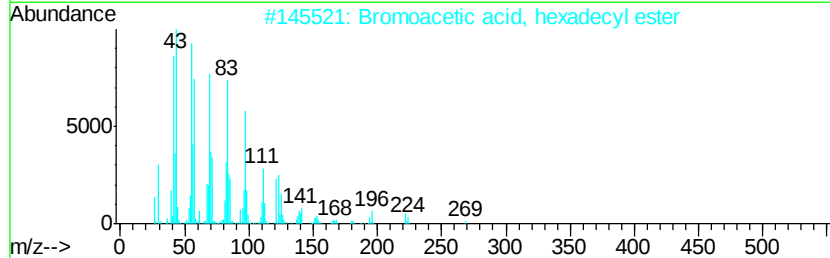
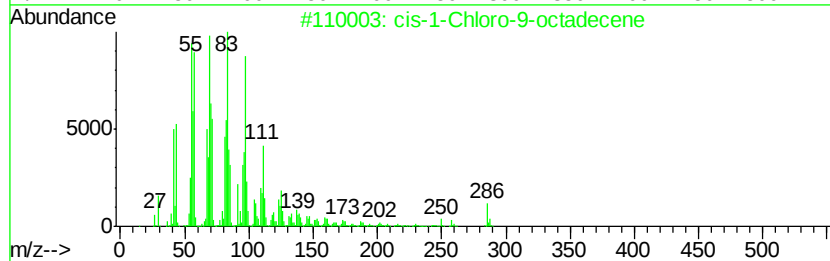
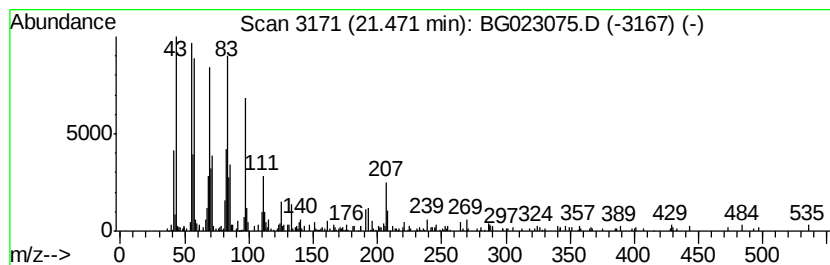
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Peak Number 6 cis-1-Chloro-9-octadecene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.47	2.24 ng	295265	Chrysene-d12	21.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	cis-1-Chloro-9-octadecene	286	C18H35Cl	016507-61-2	90
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	87
3		1-Hexacosanol	382	C26H54O	000506-52-5	87
4		Cyclotetradecane	196	C14H28	000295-17-0	87
5		1-Tetradecene	196	C14H28	001120-36-1	86



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TIC Library : C:\DATABASE\NIST02.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown3.04	3.04	281.7	ng	9425710	1	8.16	669109	20.0
2-Pentanone, 4-hy...	5.23	19.0	ng	635943	1	8.16	669109	20.0
unknown7.68	7.68	102.2	ng	3417480	1	8.16	669109	20.0
n-Hexadecanoic acid	18.43	4.2	ng	521456	4	17.56	2484980	20.0
cis-1-Chloro-9-oc...	21.47	2.2	ng	295265	5	21.86	2635320	20.0