

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041715\
 Data File : BG016515.D
 Acq On : 18 Apr 2015 9:29
 Operator : TP/IZ
 Sample : G1855-09
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LS-SB14A

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-BG040615.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	2.753	6	11	20	rBV	110253	198634	7.90%	1.144%
2	2.830	20	24	29	rVV	96422	125833	5.01%	0.725%
3	2.877	29	32	40	rVB	20004	26813	1.07%	0.154%
4	4.775	348	355	362	rBV	127231	175705	6.99%	1.012%
5	5.250	430	436	453	rVB	975536	1368837	54.46%	7.883%
6	6.849	700	708	721	rBV	994868	1511212	60.12%	8.703%
7	6.960	723	727	736	rVB	20476	35273	1.40%	0.203%
8	7.195	760	767	779	rBV	1012737	1543706	61.42%	8.890%
9	7.659	838	846	855	rBV	214609	338050	13.45%	1.947%
10	7.977	893	900	910	rVB	742189	1148659	45.70%	6.615%
11	8.817	1034	1043	1054	rBV	540405	868243	34.54%	5.000%
12	10.444	1312	1320	1326	rBV	303085	503804	20.04%	2.901%
13	12.918	1734	1741	1755	rBV	1330600	1931050	76.83%	11.120%
14	13.758	1879	1884	1893	rBV	74399	114012	4.54%	0.657%
15	14.299	1970	1976	1983	rBV2	434841	673106	26.78%	3.876%
16	15.791	2224	2230	2239	rBV	864099	1212751	48.25%	6.984%
17	16.014	2264	2268	2270	rBV	22307	27750	1.10%	0.160%
18	17.043	2437	2443	2448	rBV2	610007	847149	33.70%	4.879%
19	17.084	2448	2450	2456	rVB2	26199	29874	1.19%	0.172%
20	17.166	2462	2464	2471	rVB3	22715	31946	1.27%	0.184%
21	19.105	2790	2794	2799	rVB	31140	41920	1.67%	0.241%
22	19.463	2849	2855	2862	rVB	32108	55150	2.19%	0.318%
23	19.669	2885	2890	2901	rVB	1944595	2513465	100.00%	14.474%
24	20.932	3102	3105	3115	rBV2	91294	129959	5.17%	0.748%
25	21.220	3148	3154	3159	rBV	733722	953713	37.94%	5.492%
26	22.777	3413	3419	3423	rBV2	22862	47295	1.88%	0.272%
27	23.453	3526	3534	3549	rVB2	469031	910944	36.24%	5.246%

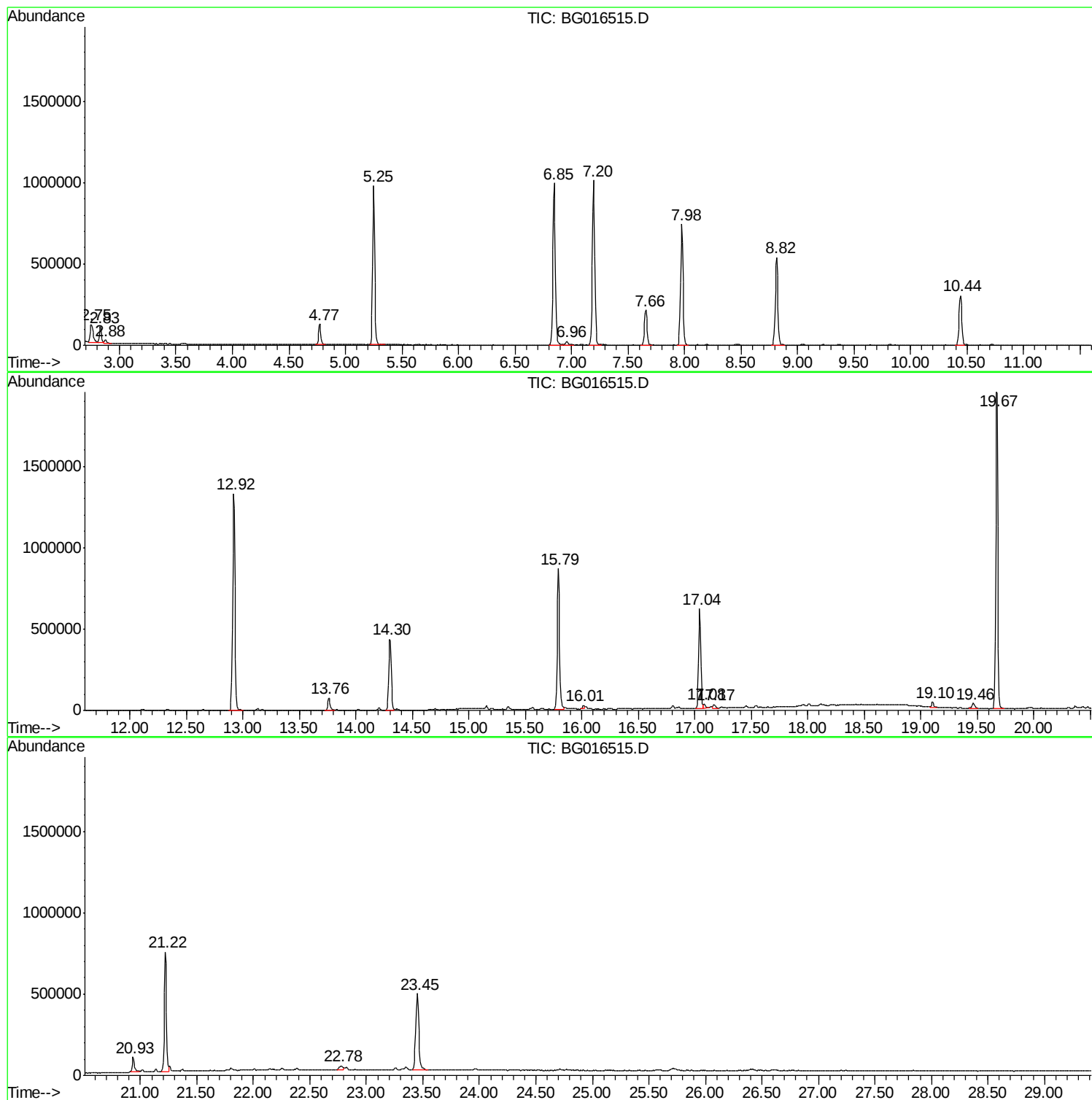
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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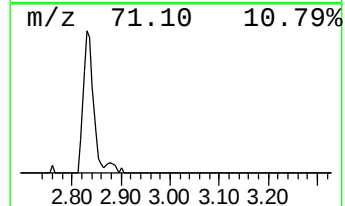
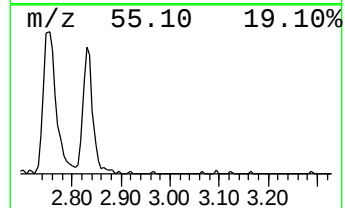
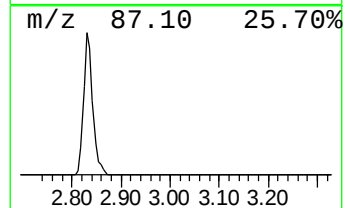
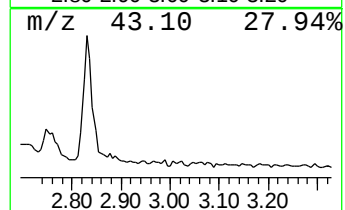
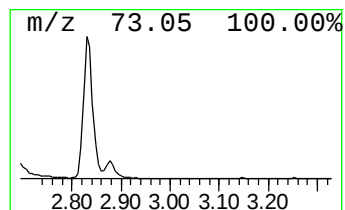
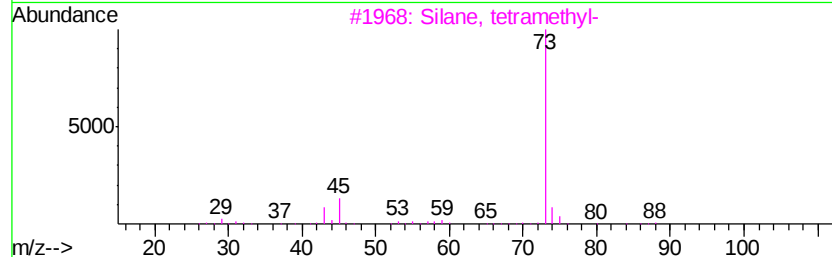
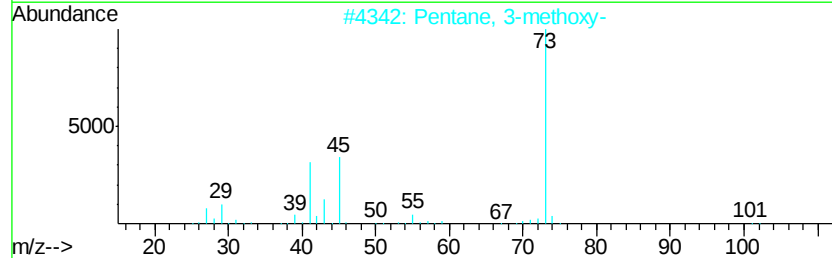
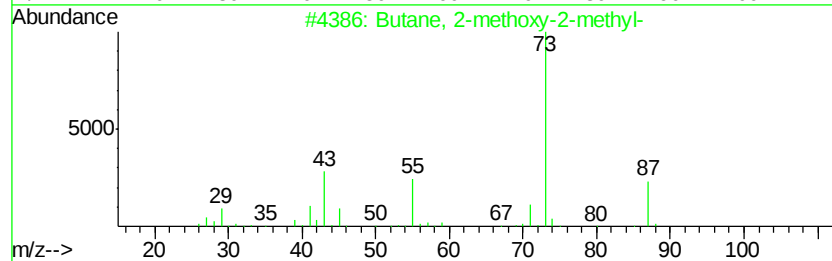
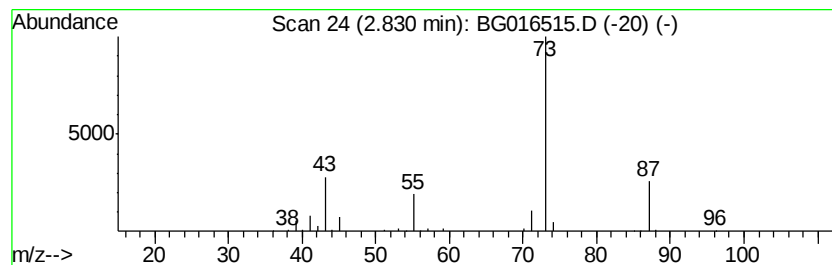
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.83	7.44 ng	125833	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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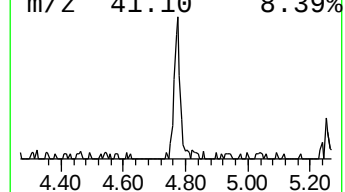
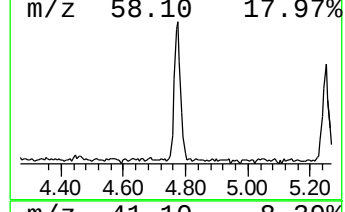
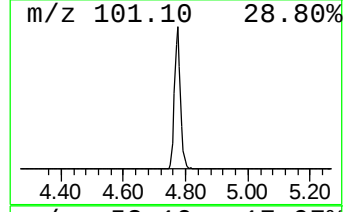
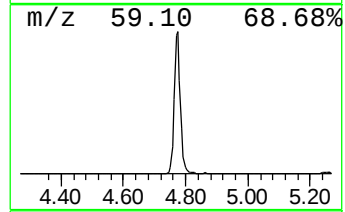
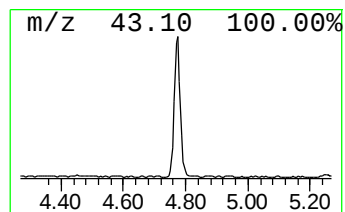
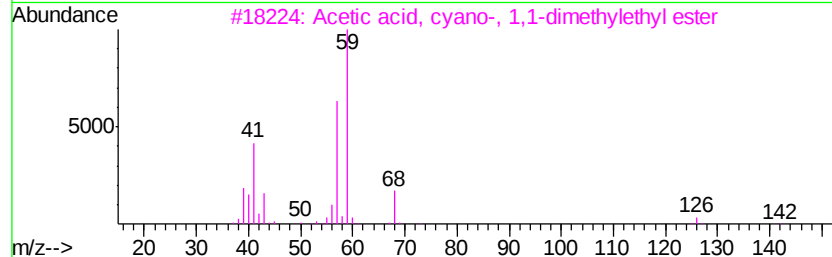
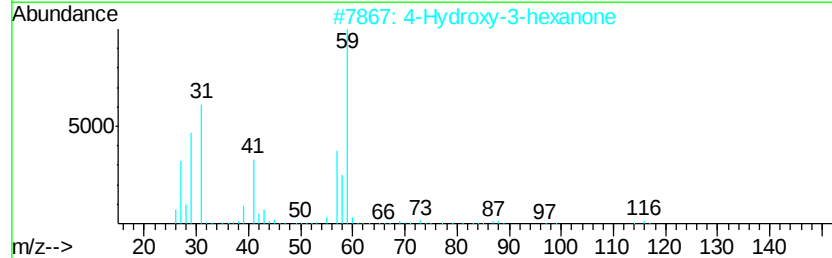
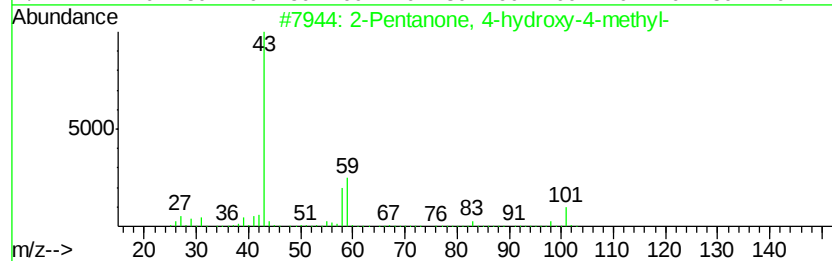
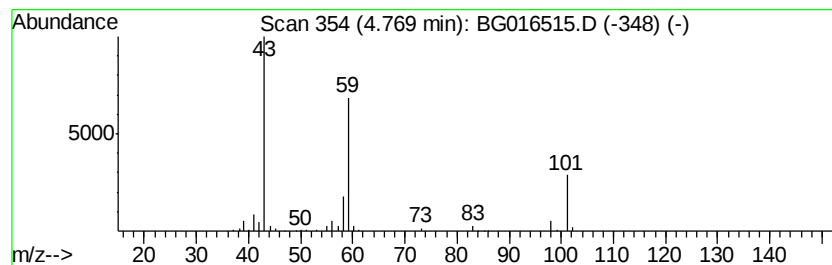
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.77	10.40 ng	175705	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4		1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	17
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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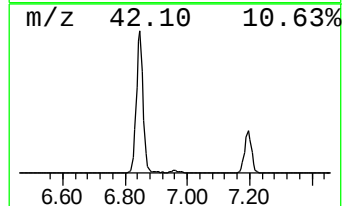
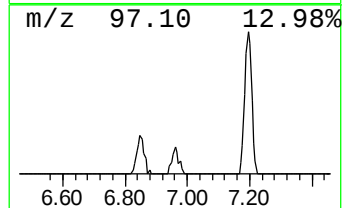
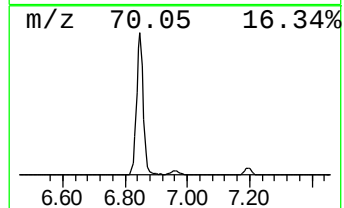
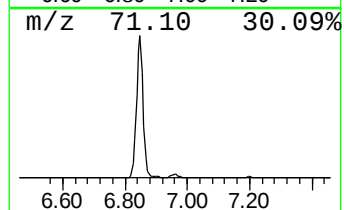
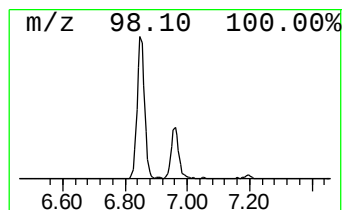
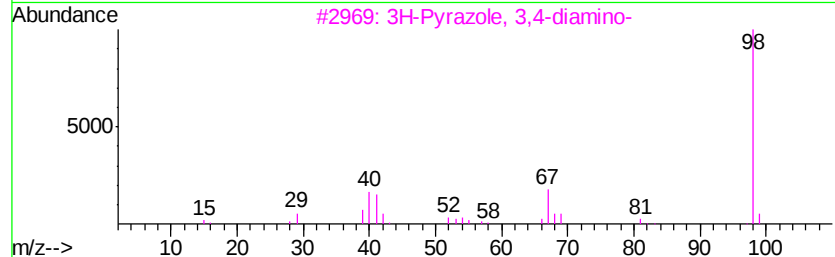
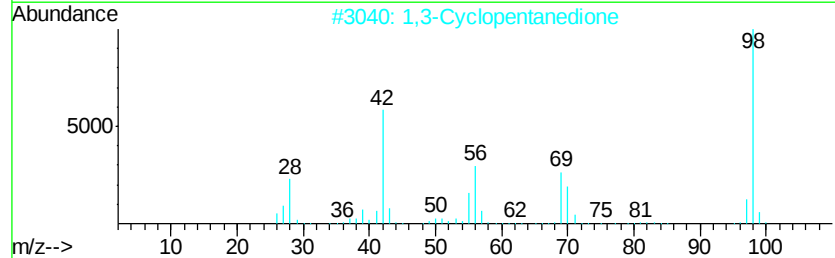
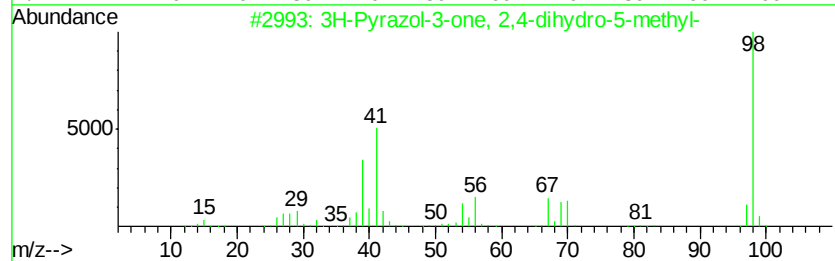
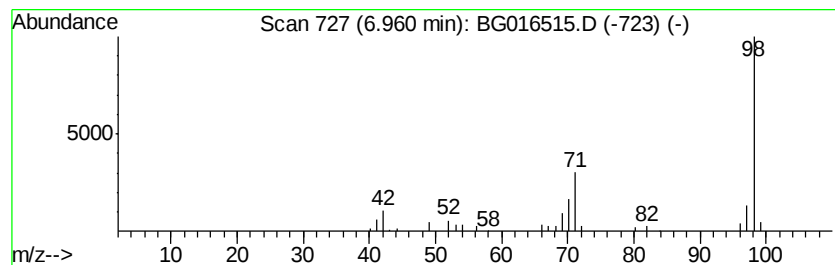
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 3H-Pyrazol-3-one, 2,4-dihyd... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.96	2.09 ng	35273	1,4-Dichlorobenzene-d4	7.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3H-Pyrazol-3-one, 2,4-dihydro-5-...	98	C4H6N2O	000108-26-9	59
2		1,3-Cyclopentanedione	98	C5H6O2	003859-41-4	59
3		3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	50
4		Benzen-d5-amine	98	C6H2D5N	004165-61-1	50
5		3H-Pyrazol-3-one, 1,2-dihydro-5-...	98	C4H6N2O	004344-87-0	45



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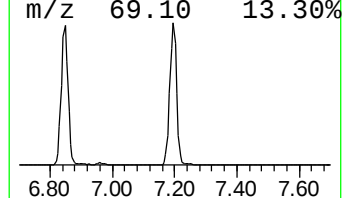
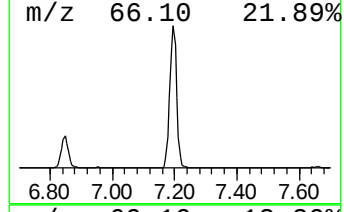
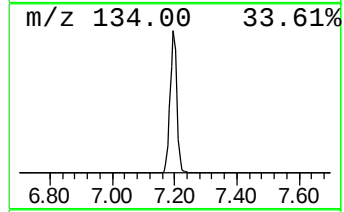
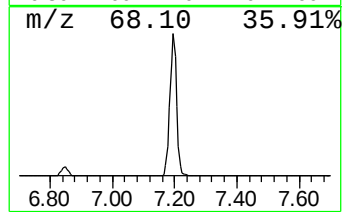
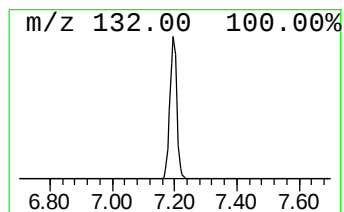
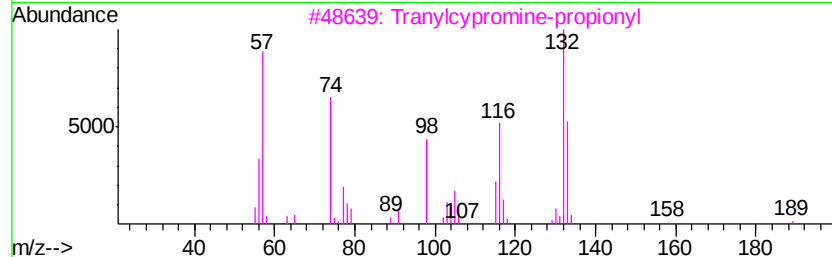
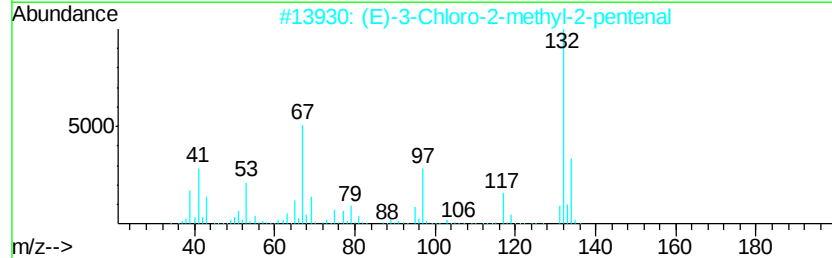
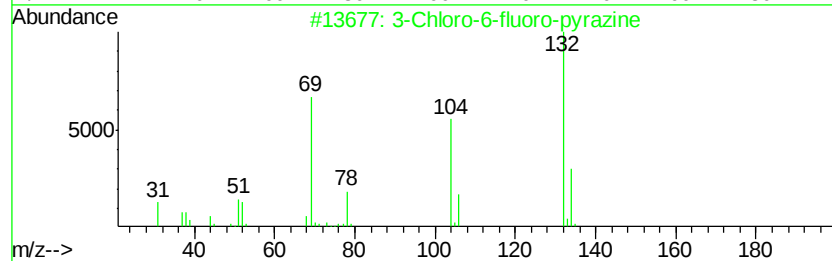
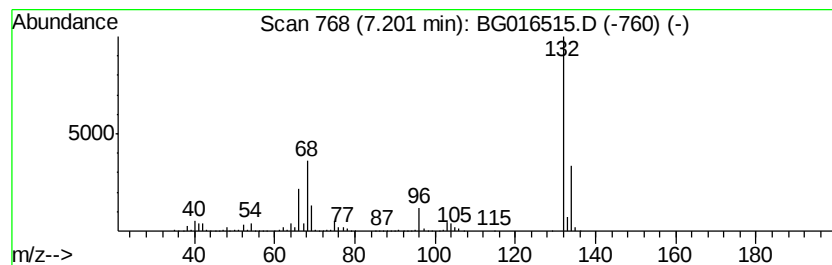
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Peak Number 5 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	91.33 ng	1543710	1,4-Dichlorobenzene-d4	7.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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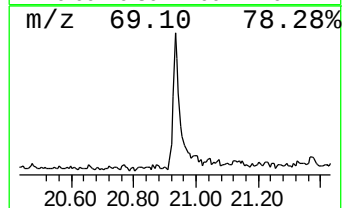
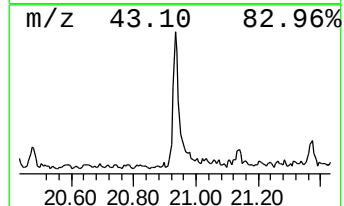
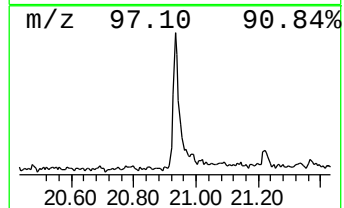
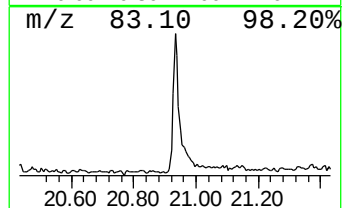
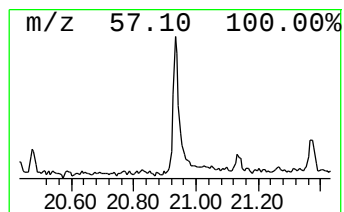
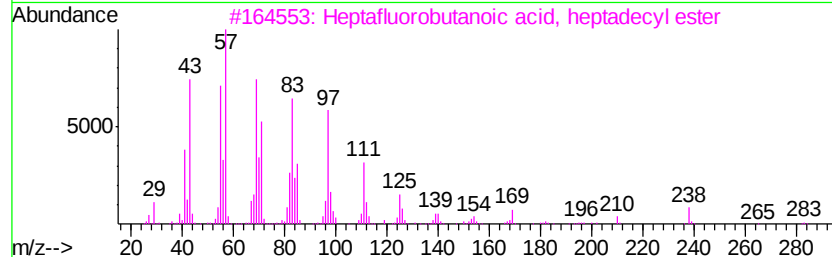
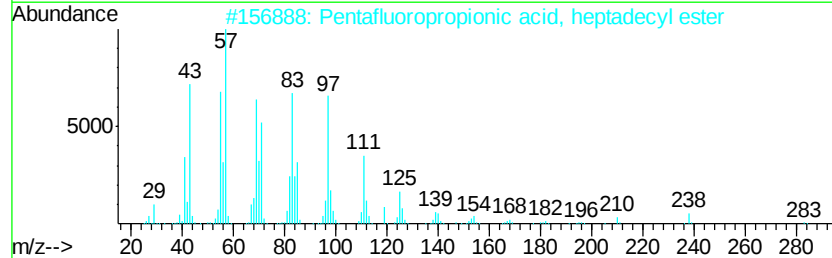
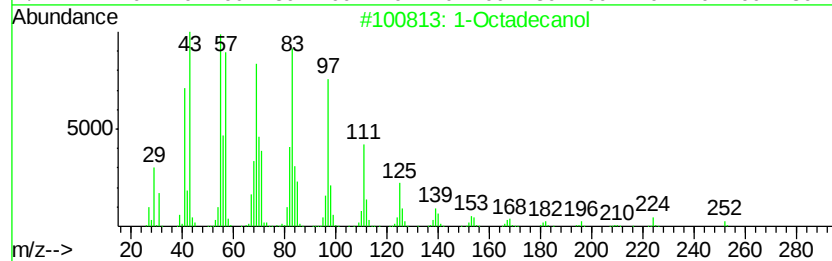
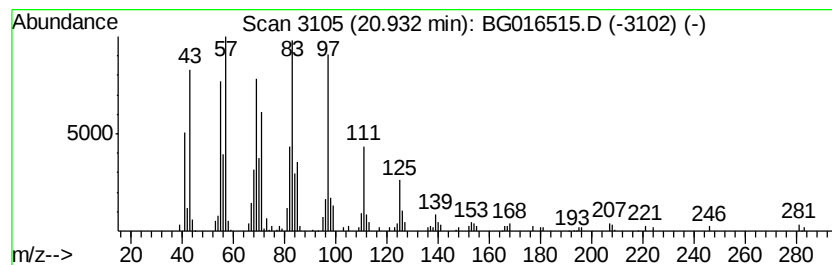
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Peak Number 7 1-Octadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.93	2.73 ng	129959	Chrysene-d12	21.22
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Octadecanol	270 C18H38O	000112-92-5	90
2	Pentafluoropropionic acid, hepta...	402 C20H35F5O2	1000283-04-2	76
3	Heptafluorobutanoic acid, heptad...	452 C21H35F7O2	1000282-97-3	68
4	Heptafluorobutyric acid, n-octad...	466 C22H37F7O2	000400-57-7	64
5	Trifluoroacetic acid, n-octadecy...	366 C20H37F3O2	079392-43-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.83	7.4	ng	125833	1	7.66	338050	20.0
2-Pentanone, 4-hy...	4.77	10.4	ng	175705	1	7.66	338050	20.0
3H-Pyrazol-3-one, ...	6.96	2.1	ng	35273	1	7.66	338050	20.0
unknown7.20	7.20	91.3	ng	1543710	1	7.66	338050	20.0
1-Octadecanol	20.93	2.7	ng	129959	5	21.22	953713	20.0