

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG110119\
 Data File : BG043469.D
 Acq On : 1 Nov 2019 17:19
 Operator : JU
 Sample : K5603-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 20190948-COMPOSITE-KM-PA

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG102119.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	3.181	11	16	25	rVB2	99394	158642	9.20%	1.275%
2	5.114	340	345	361	rVB	101013	164619	9.54%	1.323%
3	5.602	421	428	440	rBV	501756	886372	51.39%	7.126%
4	7.194	692	699	711	rBV	518993	985769	57.15%	7.925%
5	7.306	714	718	729	rVB	24700	51124	2.96%	0.411%
6	7.553	751	760	770	rBV	557407	999219	57.93%	8.033%
7	8.011	831	838	848	rBV	133476	238463	13.83%	1.917%
8	8.340	884	894	905	rBV	321897	594767	34.48%	4.782%
9	9.174	1027	1036	1054	rBV	242087	518107	30.04%	4.165%
10	10.820	1308	1316	1326	rBV	147595	306822	17.79%	2.467%
11	13.264	1725	1732	1747	rBV	589510	998836	57.91%	8.030%
12	14.092	1866	1873	1885	rBV	80055	148188	8.59%	1.191%
13	14.639	1960	1966	1982	rBV	295785	494679	28.68%	3.977%
14	16.131	2213	2220	2235	rBV	784476	1354555	78.53%	10.890%
15	17.388	2427	2434	2445	rBV	370792	641385	37.19%	5.157%
16	17.506	2449	2454	2459	rVB3	17797	27827	1.61%	0.224%
17	18.275	2580	2585	2594	rBV8	20760	44437	2.58%	0.357%
18	19.997	2872	2878	2895	rBV	1215842	1724792	100.00%	13.867%
19	21.290	3093	3098	3107	rBV8	30839	65056	3.77%	0.523%
20	21.654	3153	3160	3177	rVB	426840	809189	46.92%	6.506%
21	22.435	3291	3293	3300	rVB5	17689	26261	1.52%	0.211%
22	23.129	3406	3411	3417	rVB5	26176	46994	2.72%	0.378%
23	23.317	3437	3443	3449	rVB3	48558	93787	5.44%	0.754%
24	23.916	3540	3545	3552	rVB3	34014	62879	3.65%	0.506%
25	24.321	3609	3614	3621	rVB10	15171	31011	1.80%	0.249%
26	24.844	3692	3703	3713	rBV3	302367	906692	52.57%	7.290%
27	25.972	3888	3895	3903	rVB5	20940	57810	3.35%	0.465%

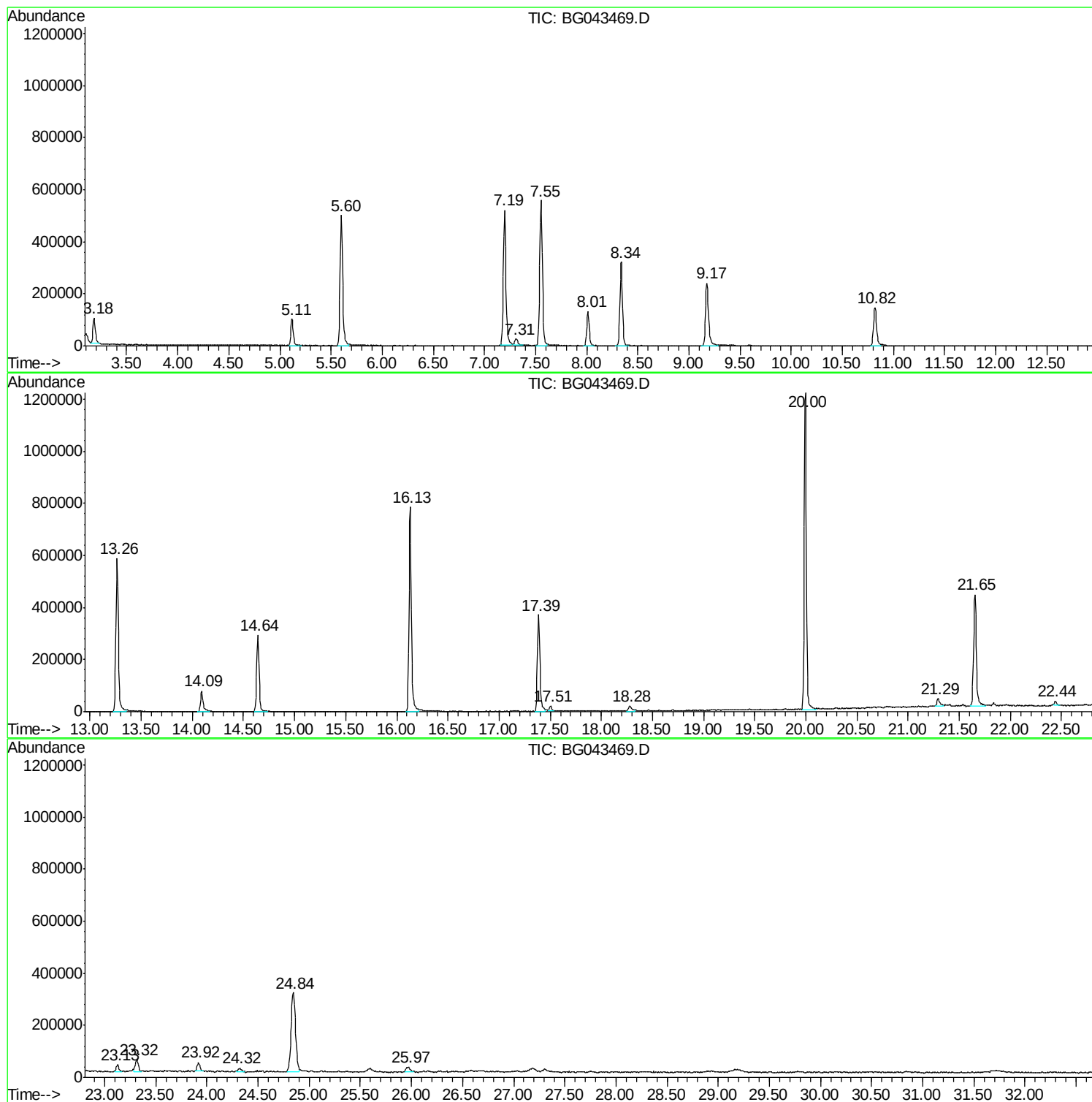
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG102119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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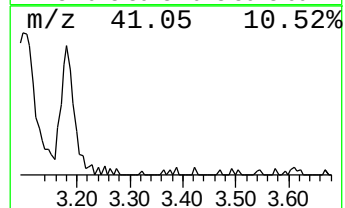
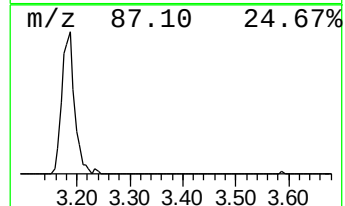
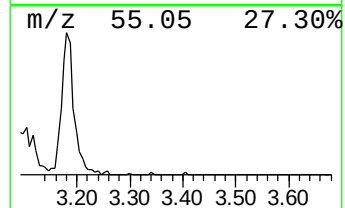
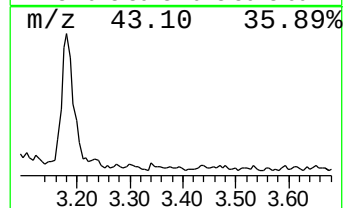
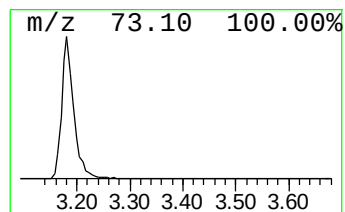
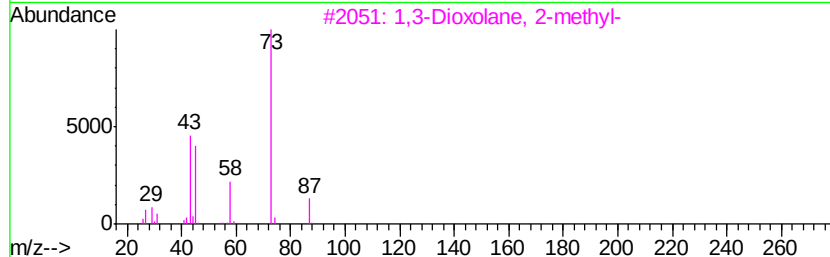
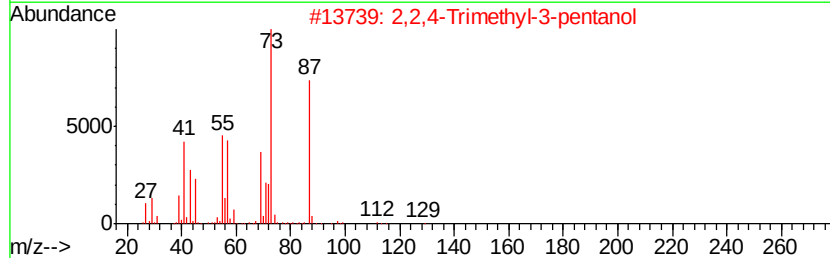
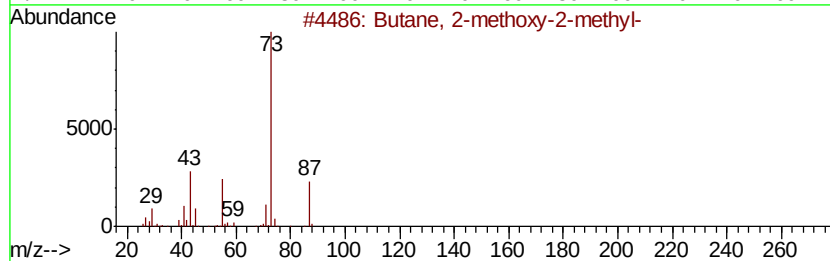
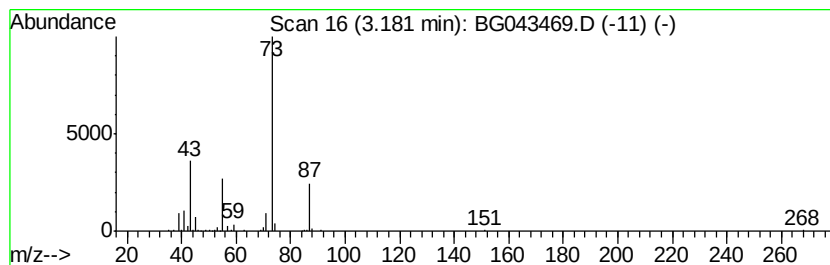
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	13.31 ng	158642	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9



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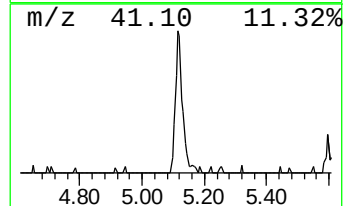
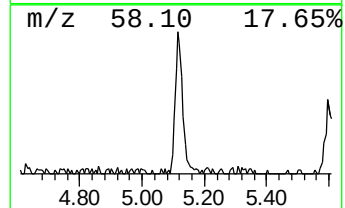
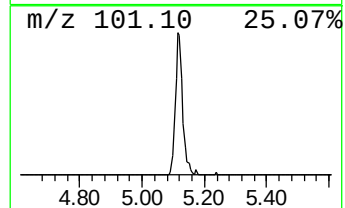
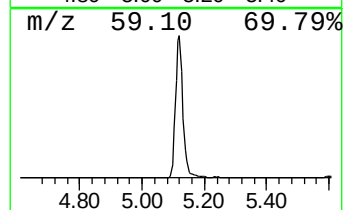
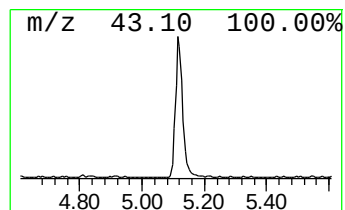
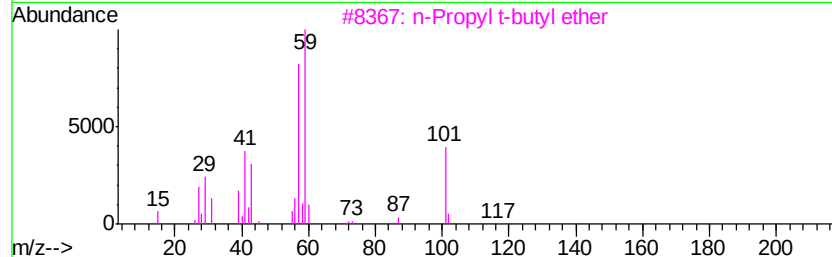
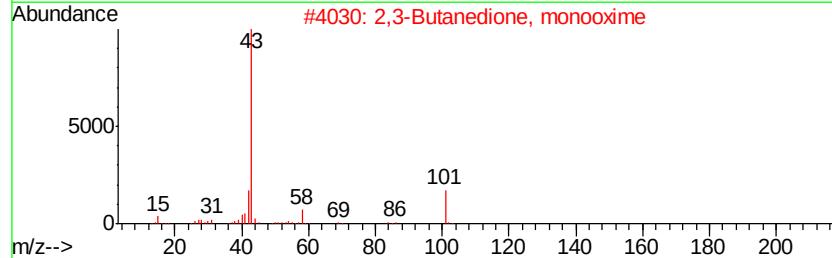
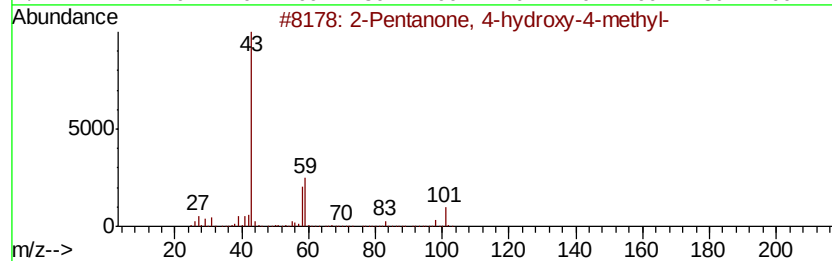
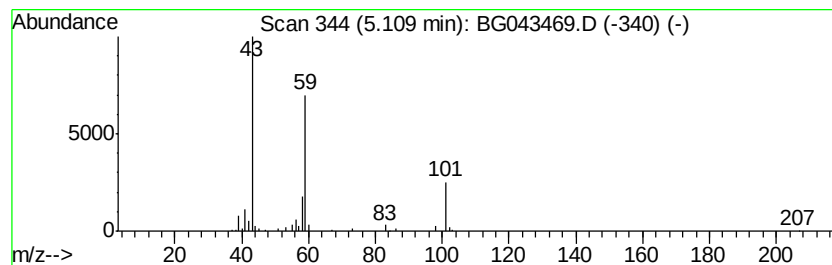
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.81 ng	164619	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
3		n-Propyl t-butyl ether	116	C7H16O	1000334-81-9	33
4		Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
5		2,2,3,3,5,8,11-Heptamethyl-4,7,1...	348	C18H40O4Si	1000367-07-2	28



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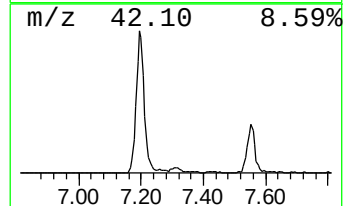
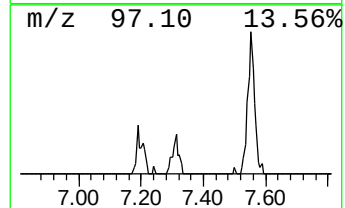
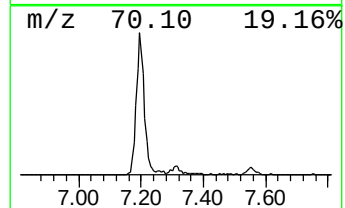
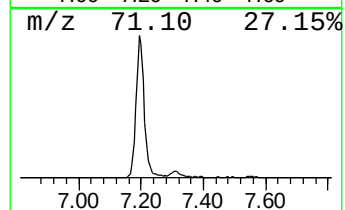
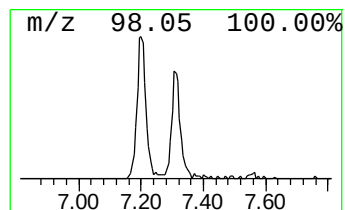
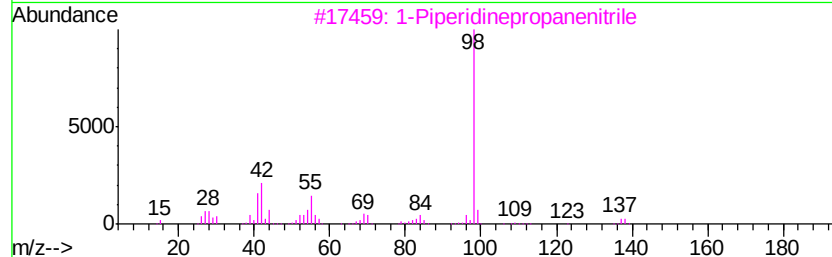
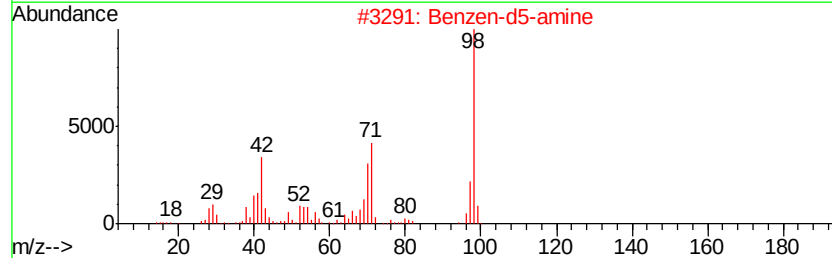
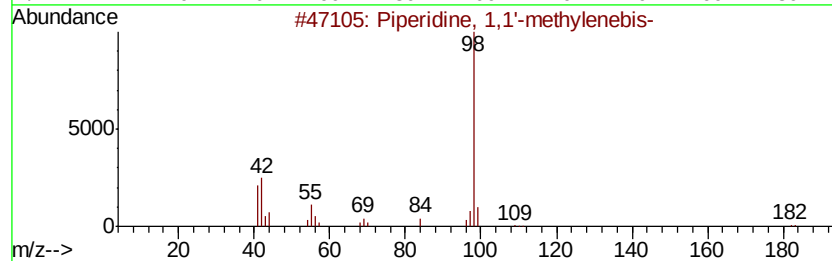
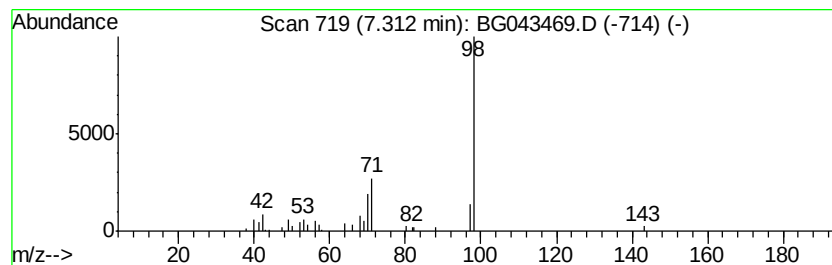
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TIC Integration Parameters: LSCINT.P

Peak Number 3 Piperidine, 1,1'-methylenebis- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.31	4.29 ng	51124	1,4-Dichlorobenzene-d4	8.01	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Piperidine, 1,1'-methylenebis-	182	C11H22N2	000880-09-1	53
2	Benzen-d5-amine	98	C6H2D5N	004165-61-1	50
3	1-Piperidinepropanenitrile	138	C8H14N2	003088-41-3	42
4	2-Pyrrolidinemethanamine, 1-ethyl-	128	C7H16N2	026116-12-1	38
5	Piperidine, 3-dimethylamino-1-me...	142	C8H18N2	1000126-80-8	36



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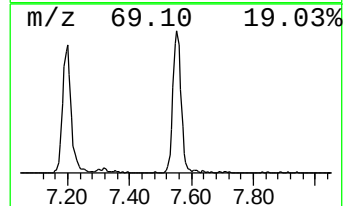
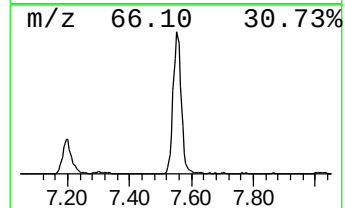
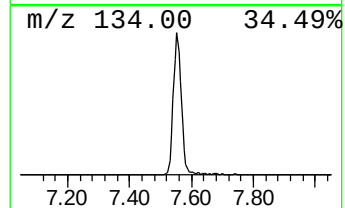
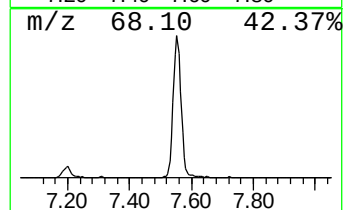
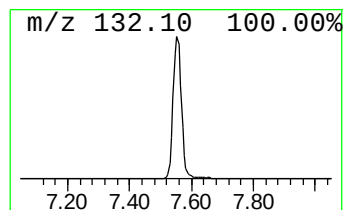
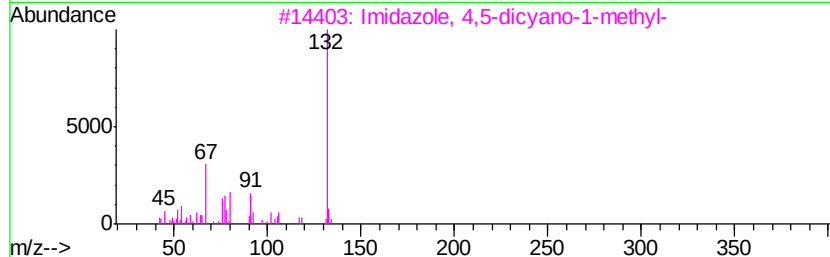
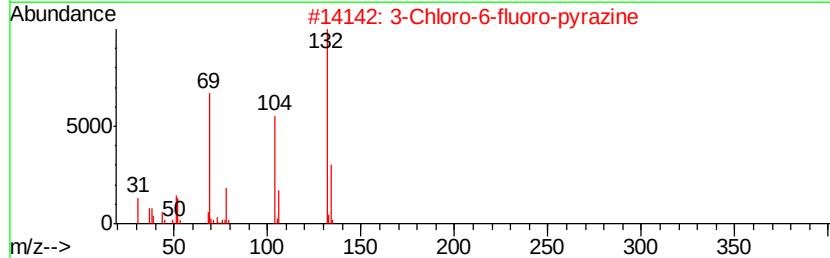
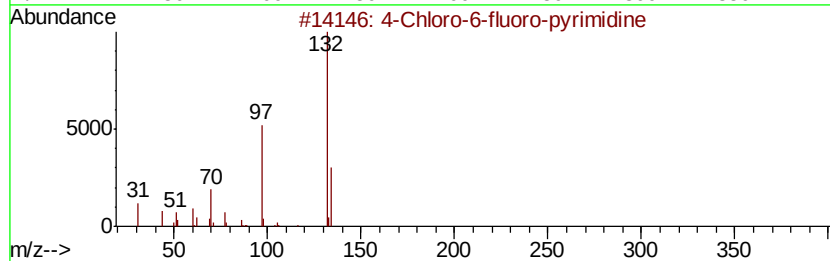
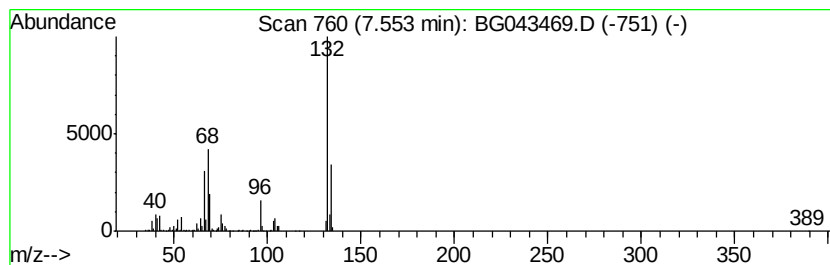
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Peak Number 4 unknown7.55 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.55	83.81 ng	999219	1,4-Dichlorobenzene-d4	8.01

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	22
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	12
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



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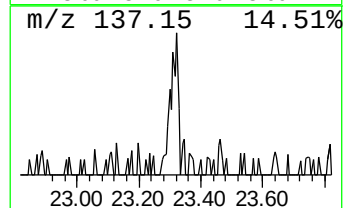
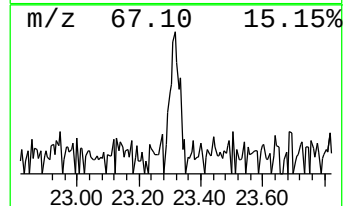
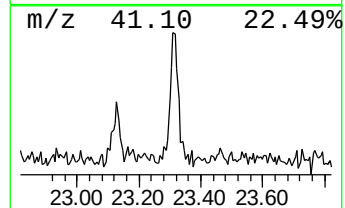
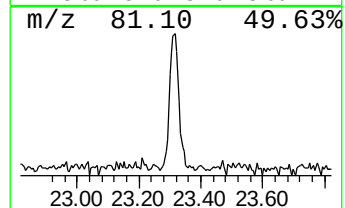
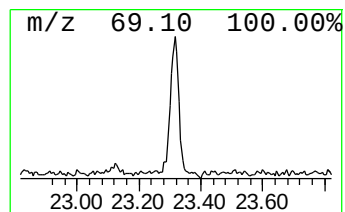
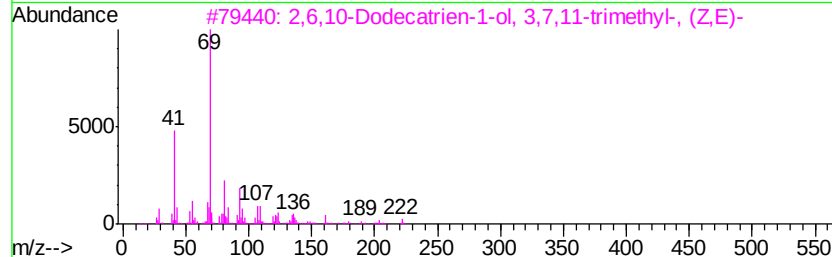
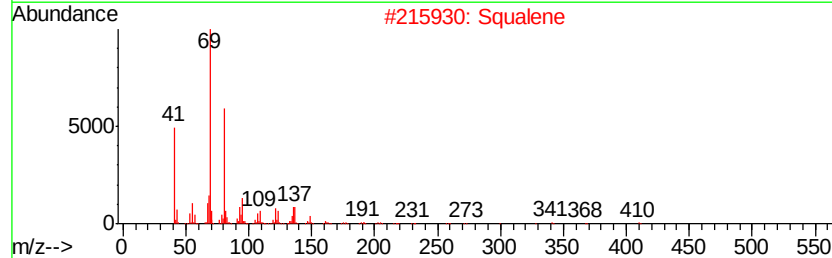
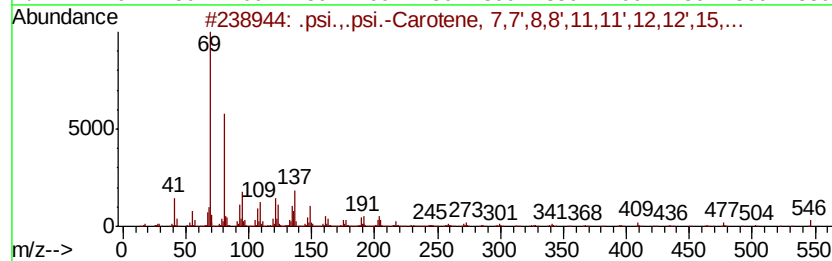
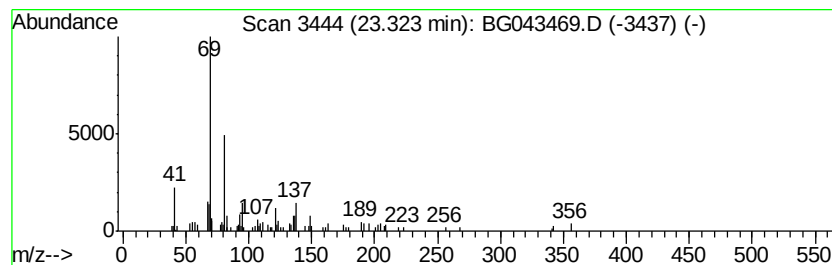
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Peak Number 6 .psi.,.psi.-Carotene, 7,7',... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.32	2.07 ng	93787	Perylene-d12	24.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	72
2		Squalene	410	C30H50	000111-02-4	64
3		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	003790-71-4	59
4		Bis(3-methylbut-3-enyl) phthalate	302	C18H22O4	022711-53-1	59
5		Pentane, 1-chloro-5-iodo-	232	C5H10ClI	060274-60-4	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.18	13.3	ng	158642	1	8.01	238463	20.0
2-Pentanone, 4-hy...	5.11	13.8	ng	164619	1	8.01	238463	20.0
Piperidine, 1,1'-...	7.31	4.3	ng	51124	1	8.01	238463	20.0
unknown7.55	7.55	83.8	ng	999219	1	8.01	238463	20.0
.psi.,.psi.-Carot...	23.32	2.1	ng	93787	6	24.84	906692	20.0