

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG011320\
 Data File : BG044026.D
 Acq On : 14 Jan 2020 00:16
 Operator : JU
 Sample : L1103-07
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-MW-19(3-5)

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-BG123019.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	3.131	3	7	27	rVB	551265	1006832	12.48%	2.132%
2	5.052	327	334	348	rBV	490246	785497	9.74%	1.663%
3	5.528	407	415	431	rBV	2055715	3467124	42.98%	7.341%
4	7.120	676	686	702	rBV	2166149	4084821	50.63%	8.649%
5	7.484	739	748	765	rBV	2163617	3904717	48.40%	8.268%
6	7.948	819	827	835	rBV	401147	709977	8.80%	1.503%
7	8.272	871	882	891	rBV	1673408	3008343	37.29%	6.370%
8	9.100	1014	1023	1036	rBV	1282545	2377761	29.47%	5.035%
9	10.745	1296	1303	1314	rBV	543355	982765	12.18%	2.081%
10	13.201	1713	1721	1737	rBV	3274561	5415377	67.13%	11.466%
11	14.029	1855	1862	1872	rBV	302085	464775	5.76%	0.984%
12	14.576	1946	1955	1965	rBV2	881128	1398971	17.34%	2.962%
13	16.062	2201	2208	2223	rBV	2817420	4443643	55.08%	9.409%
14	17.320	2415	2422	2434	rBV	1124302	1704878	21.13%	3.610%
15	19.940	2861	2868	2879	rBV	4974856	8067541	100.00%	17.082%
16	21.233	3084	3088	3101	rBV	572481	914099	11.33%	1.936%
17	21.568	3138	3145	3157	rBV	1052364	1823016	22.60%	3.860%
18	22.384	3279	3284	3293	rBV2	66024	145333	1.80%	0.308%
19	23.060	3394	3399	3405	rVB	54605	94484	1.17%	0.200%
20	23.242	3424	3430	3440	rVB	125777	246268	3.05%	0.521%
21	23.847	3527	3533	3539	rBV3	59881	119305	1.48%	0.253%
22	24.693	3666	3677	3701	rBV2	461565	1959172	24.28%	4.148%
23	25.880	3875	3879	3888	rVB3	41623	103343	1.28%	0.219%

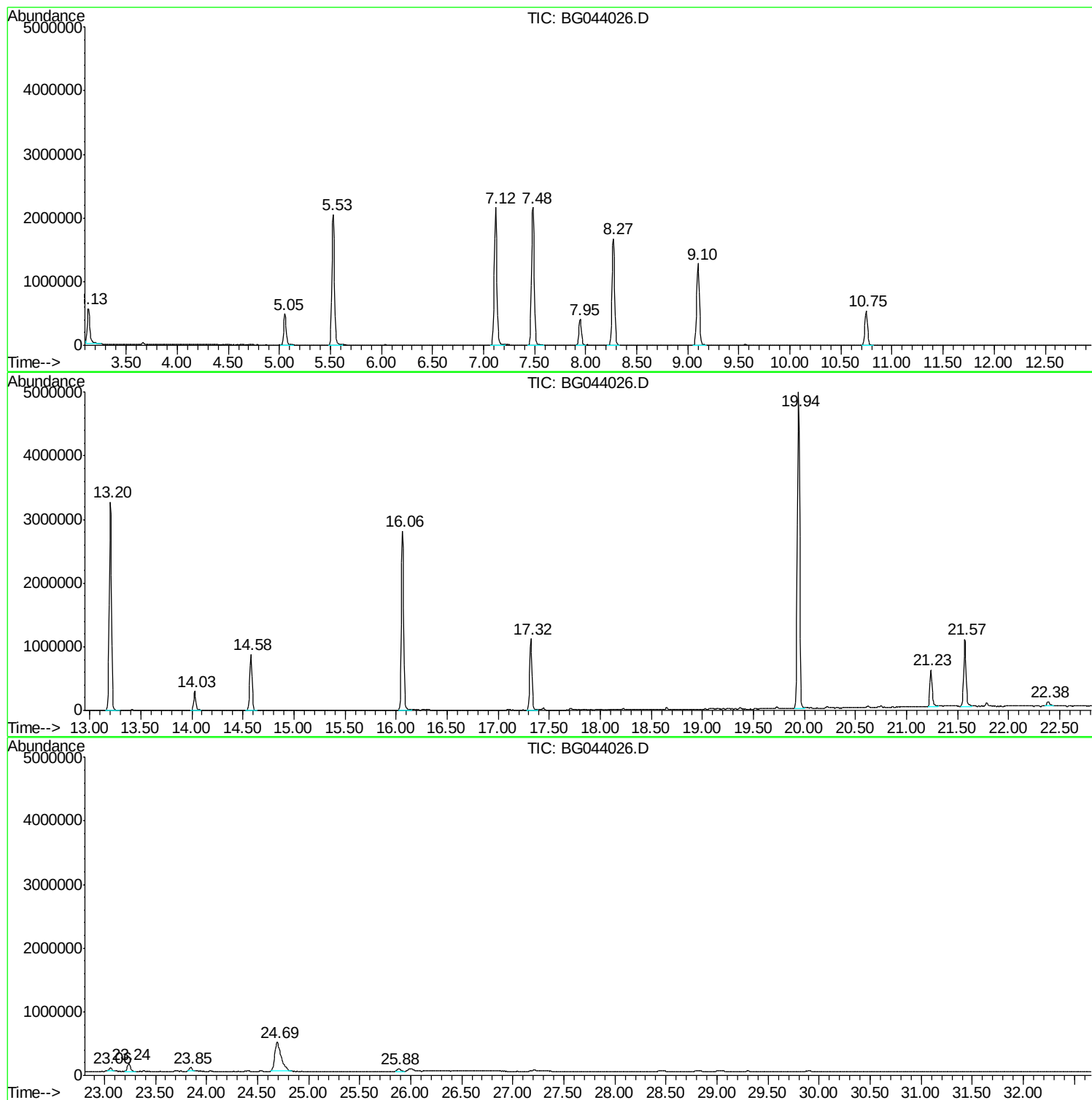
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG123019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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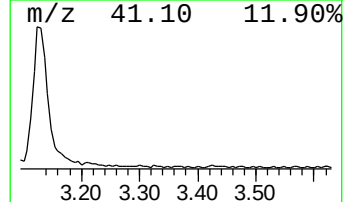
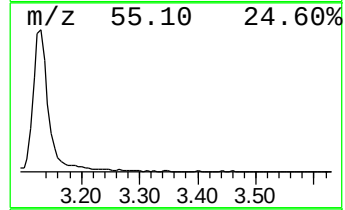
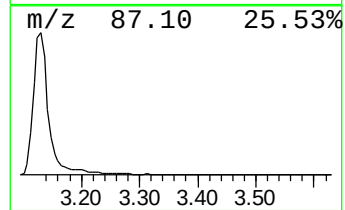
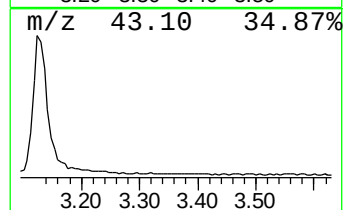
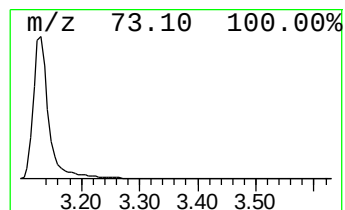
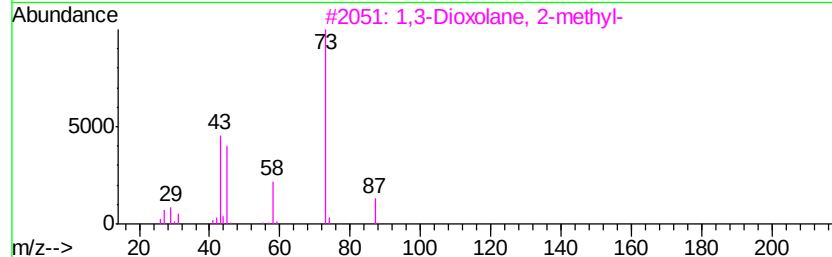
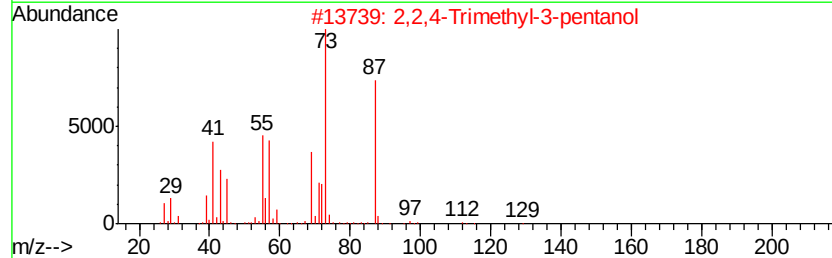
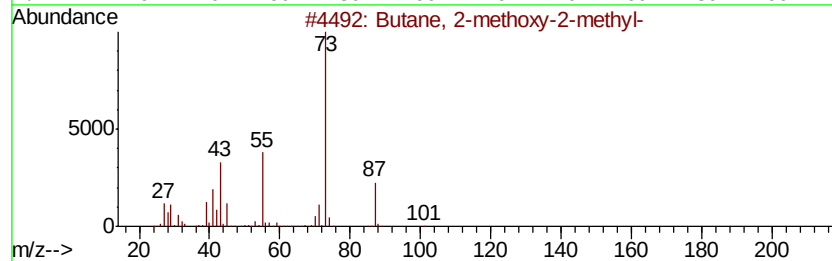
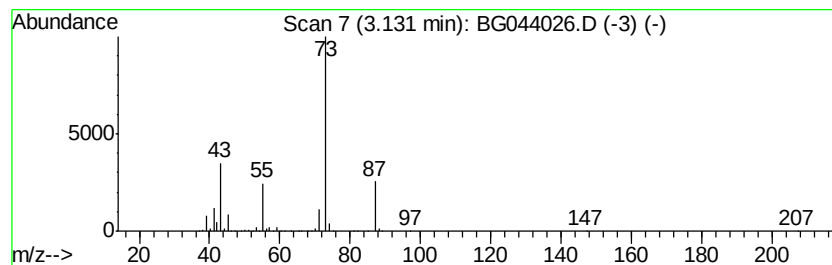
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	28.36 ng	1006830	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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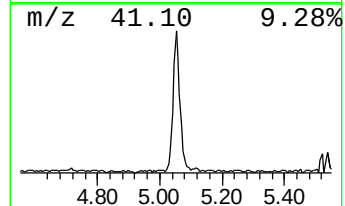
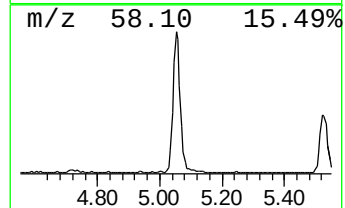
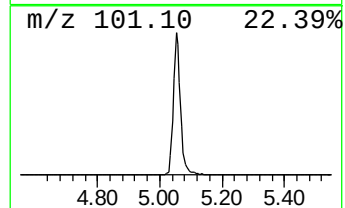
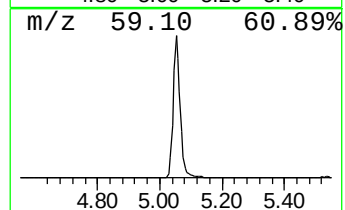
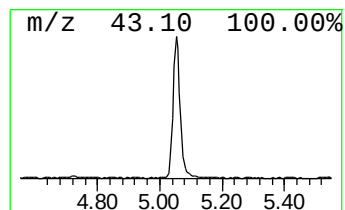
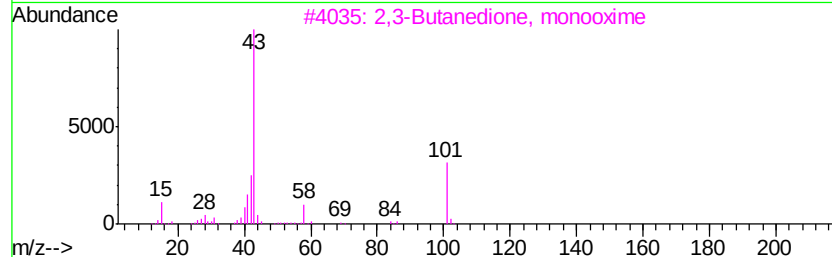
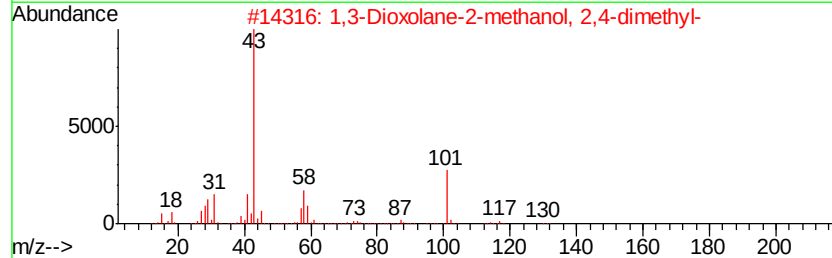
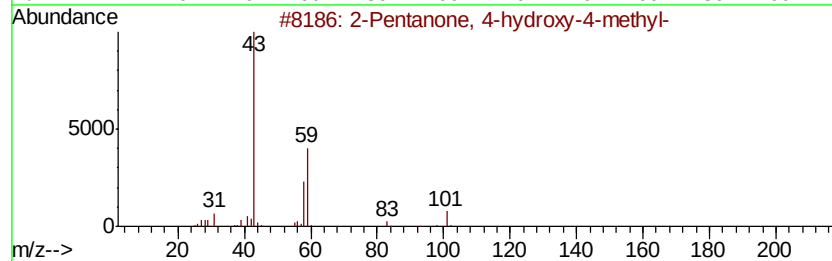
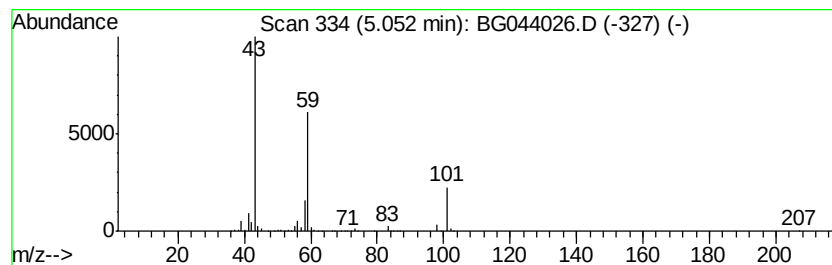
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.05	22.13 ng	785497	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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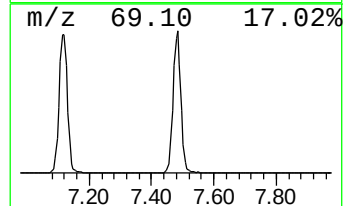
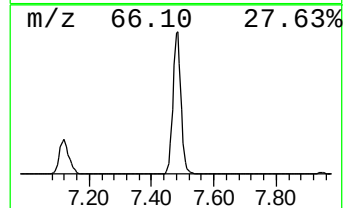
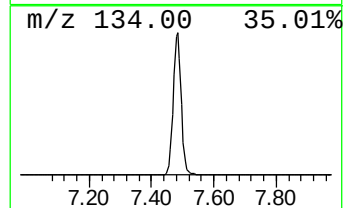
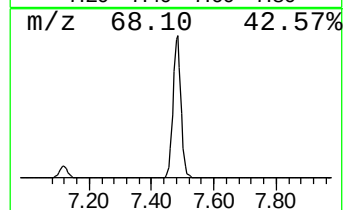
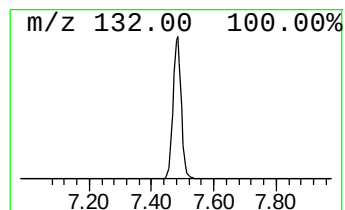
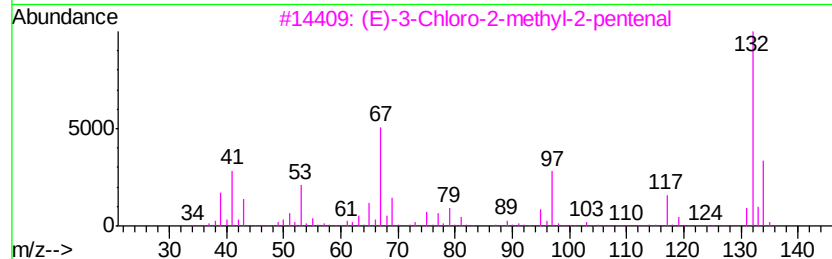
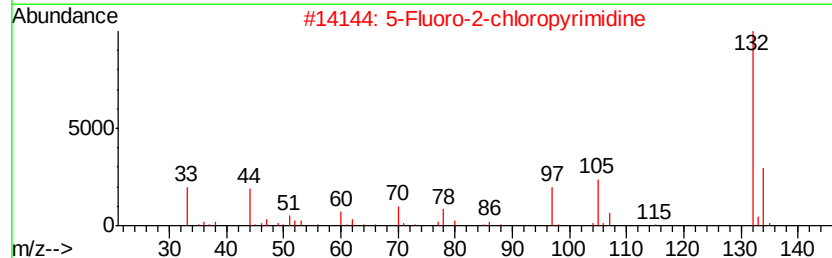
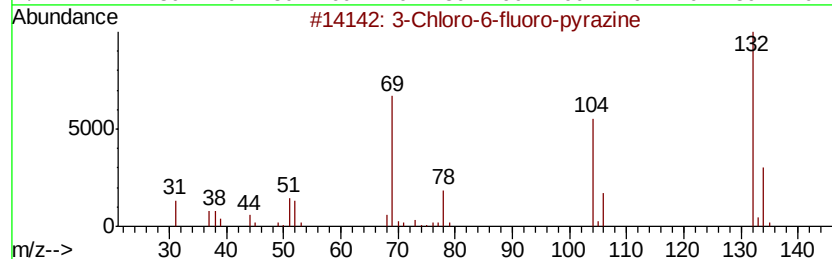
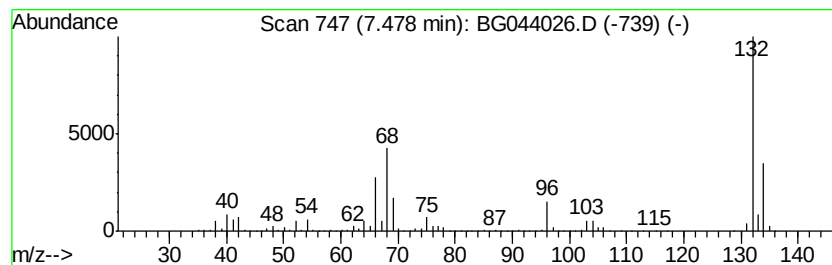
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Peak Number 3 unknown7.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.48	110.00 ng	3904720	1,4-Dichlorobenzene-d4	7.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
4		1-Isoquinolinemethanol, .alpha.-...	191	C12H17NO	114608-92-3	12
5		Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



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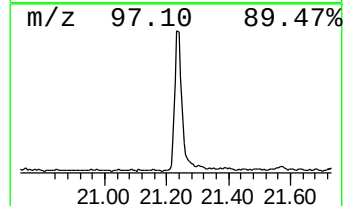
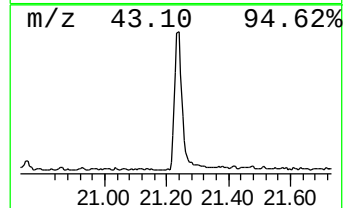
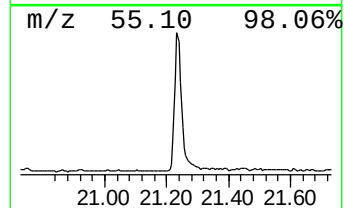
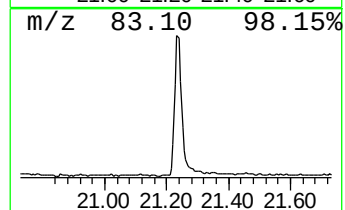
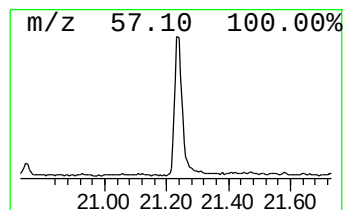
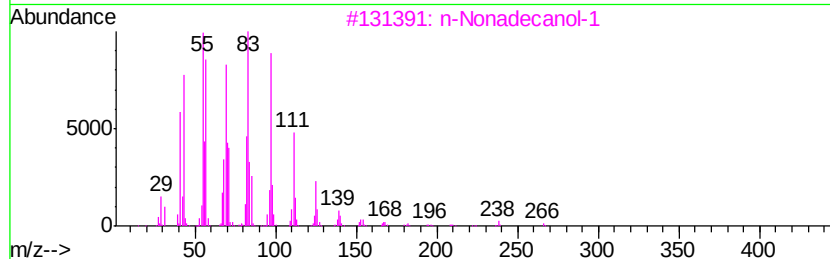
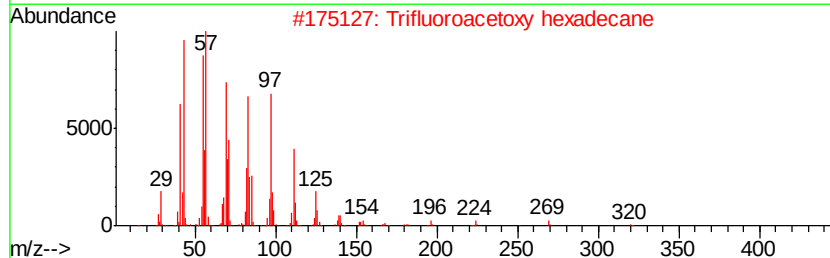
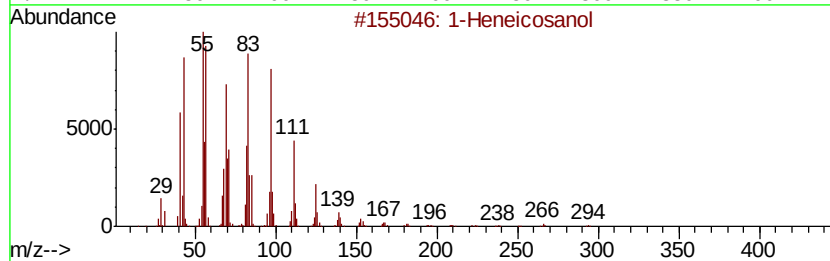
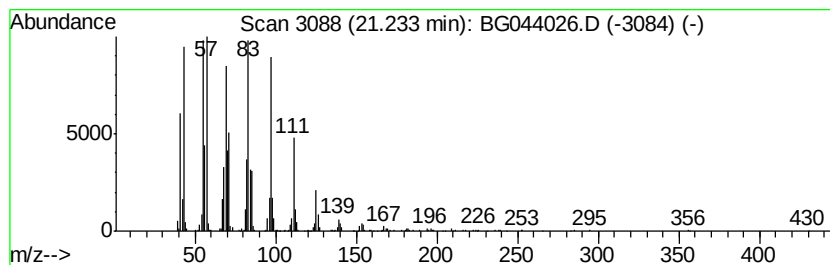
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.23	10.03 ng	914099	Chrysene-d12	21.57	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3	n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5	Behenic alcohol	326	C22H46O	000661-19-8	94



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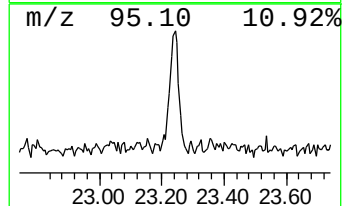
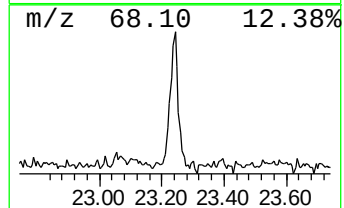
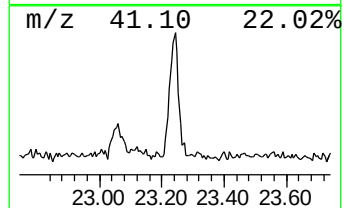
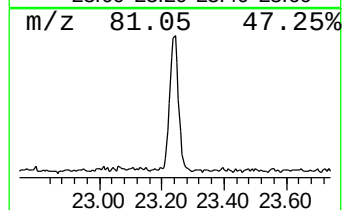
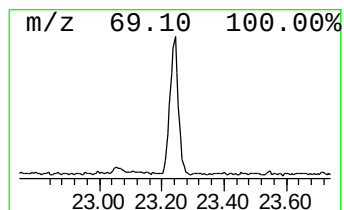
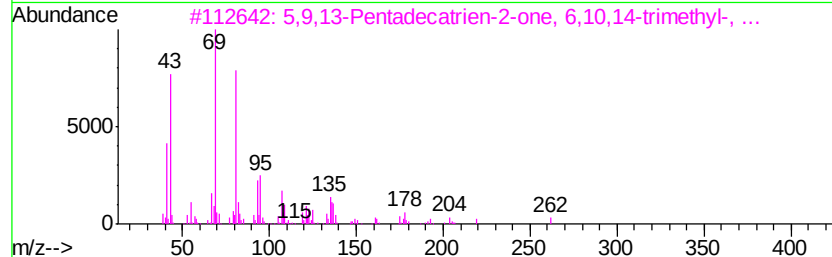
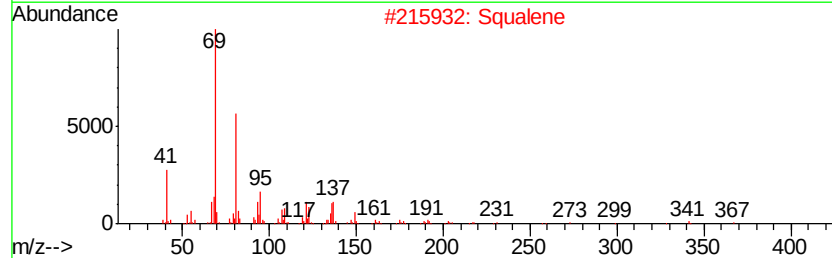
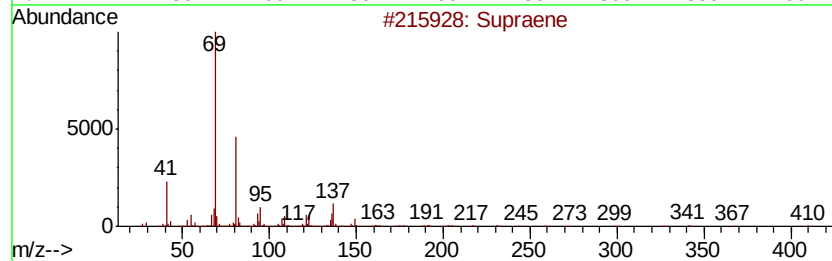
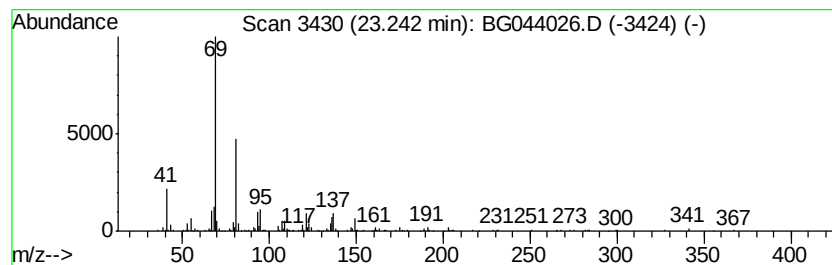
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TIC Library : C:\Database\NIST11.L
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Peak Number 6 Supraene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.24	2.51 ng	246268	Perylene-d12	24.69

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	91
3	5,9,13-Pentadecatrien-2-one, 6,1...		262	C18H30O	001117-52-8	64
4	1,5-Heptadiene, 3,3,6-trimethyl-		138	C10H18	035387-63-4	58
5	4-Oxo-.beta.-damascone		206	C13H18O2	053398-08-6	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.13	28.4	ng	1006830	1	7.95	709977	20.0
2-Pentanone, 4-hy...	5.05	22.1	ng	785497	1	7.95	709977	20.0
unknown7.48	7.48	110.0	ng	3904720	1	7.95	709977	20.0
1-Heneicosanol	21.23	10.0	ng	914099	5	21.57	1823020	20.0
Supraene	23.24	2.5	ng	246268	6	24.69	1959170	20.0