

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF031918\
 Data File : BF103782.D
 Acq On : 20 Mar 2018 3:12
 Operator : JU/SJ
 Sample : J1954-09
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 031518-TIDO-F-U-B

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_F\METHODS\8270-BF031518.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	2.298	31	36	46	rVB	378032	491172	12.88%	2.119%
2	5.198	525	529	538	rVB	93268	99086	2.60%	0.428%
3	5.586	591	595	599	rBV	1323844	1157391	30.34%	4.994%
4	5.916	648	651	660	rVB	99739	82019	2.15%	0.354%
5	6.580	760	764	768	rBV	874671	730830	19.16%	3.153%
6	6.739	786	791	794	rBV	2391956	2068894	54.23%	8.926%
7	6.969	827	830	834	rBV	895061	761474	19.96%	3.285%
8	7.127	853	857	861	rBV	2983988	2707035	70.96%	11.679%
9	7.533	921	926	929	rBV	2208917	2309103	60.53%	9.963%
10	8.251	1044	1048	1052	rBV	1189056	979375	25.67%	4.225%
11	9.327	1226	1231	1234	rBV	4082909	3814854	100.00%	16.459%
12	9.716	1293	1297	1300	rBV	121603	93210	2.44%	0.402%
13	9.927	1330	1333	1336	rBV	63095	49346	1.29%	0.213%
14	10.010	1344	1347	1351	rVB2	1126197	954516	25.02%	4.118%
15	10.427	1416	1418	1421	rVB	83127	58760	1.54%	0.254%
16	10.804	1478	1482	1485	rBV	1473972	1367477	35.85%	5.900%
17	10.904	1495	1499	1503	rVB	58816	64744	1.70%	0.279%
18	11.504	1597	1601	1604	rBV	1010387	827047	21.68%	3.568%
19	13.092	1867	1871	1875	rBV	2989503	2957146	77.52%	12.758%
20	13.974	2017	2021	2029	rBV	178812	185140	4.85%	0.799%
21	14.156	2048	2052	2055	rBV	824670	755907	19.81%	3.261%
22	15.692	2307	2313	2323	rVB	517092	663333	17.39%	2.862%

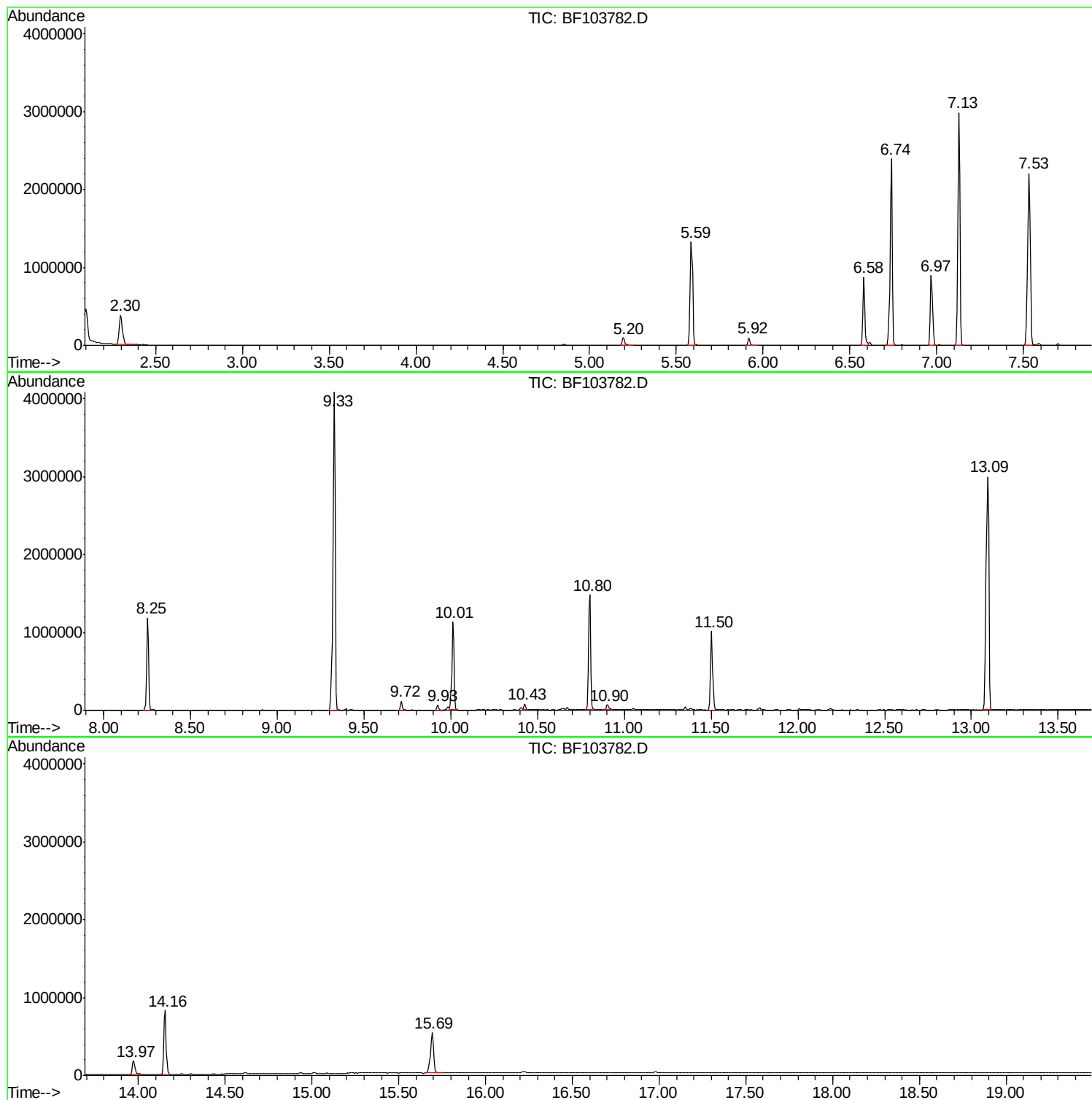
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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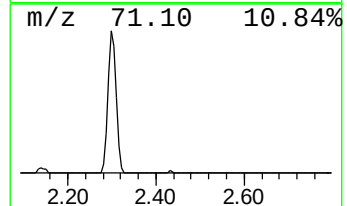
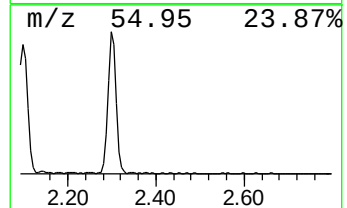
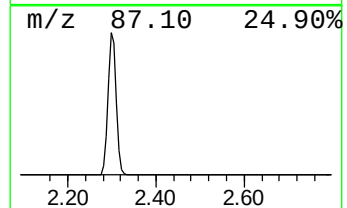
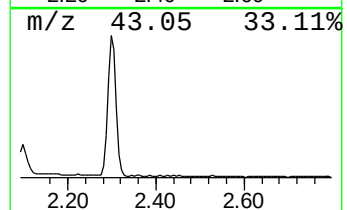
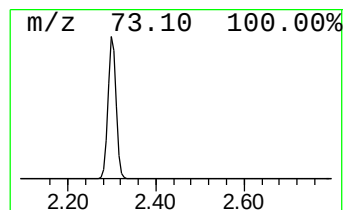
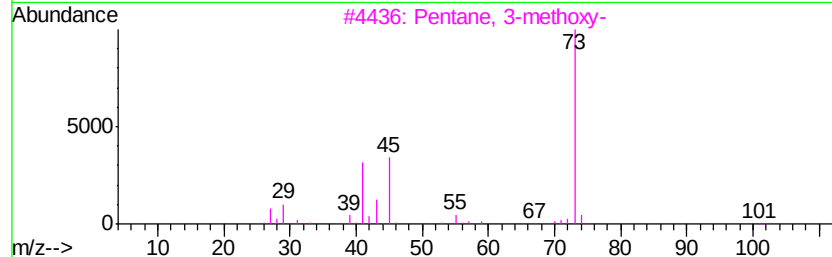
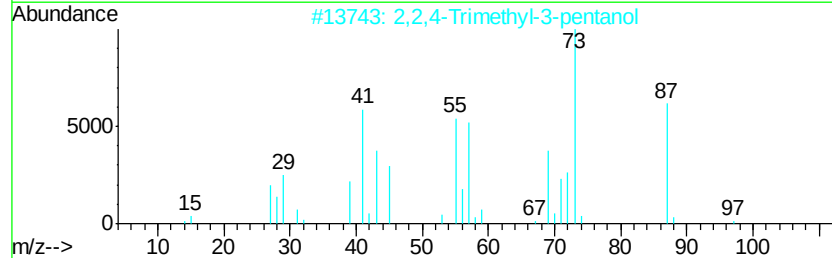
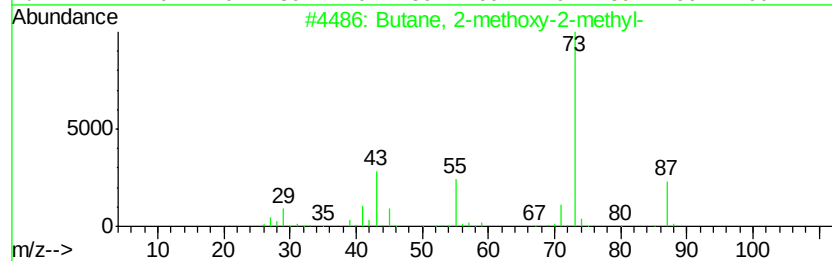
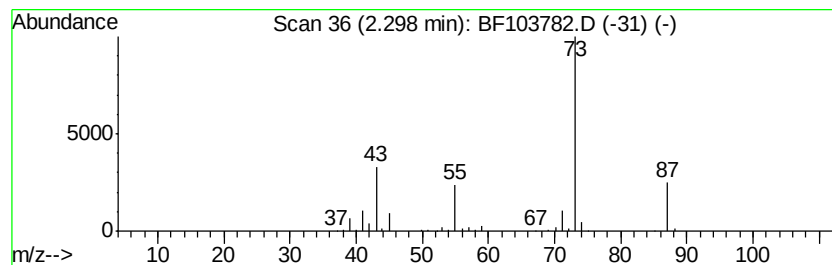
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031518.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.30	12.90 ng	491172	1,4-Dichlorobenzene-d4	6.97

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	56
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9
5		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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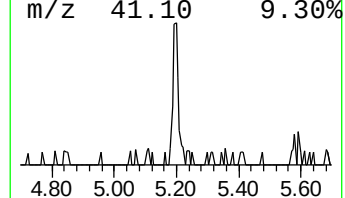
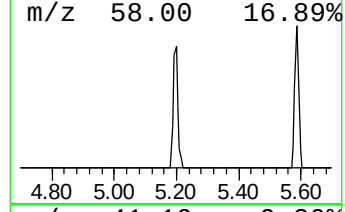
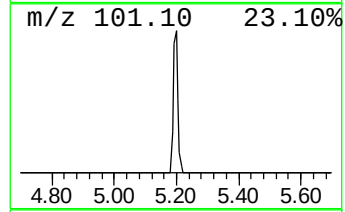
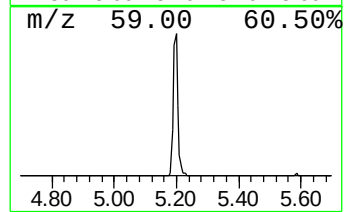
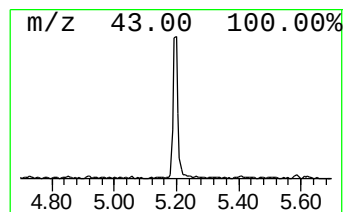
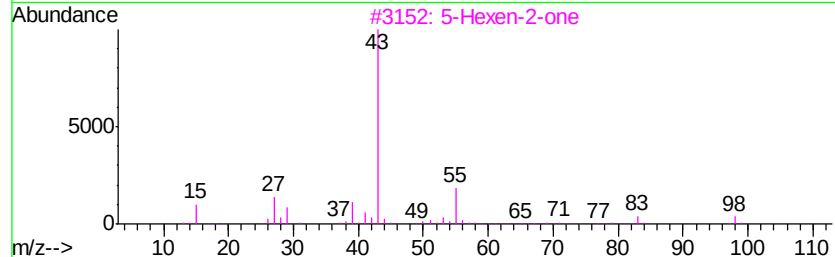
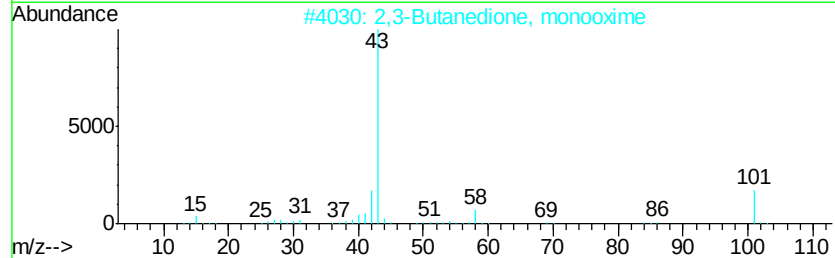
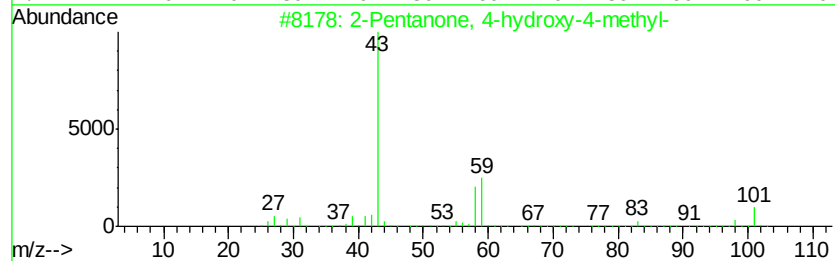
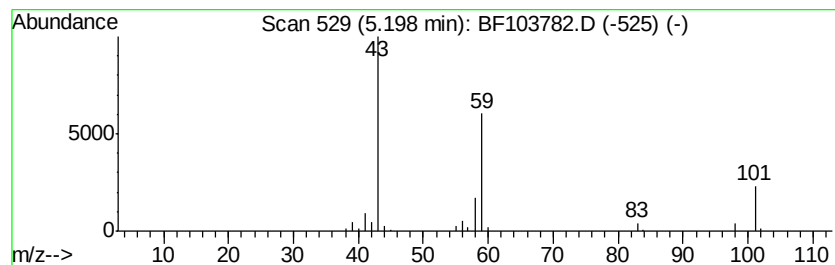
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	2.60 ng	99086	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		5-Hexen-2-one	98	C6H10O	000109-49-9	10
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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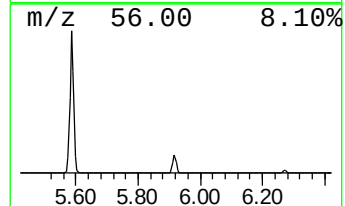
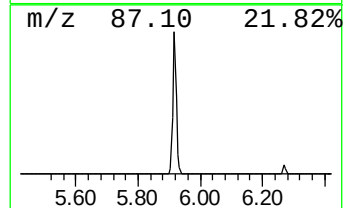
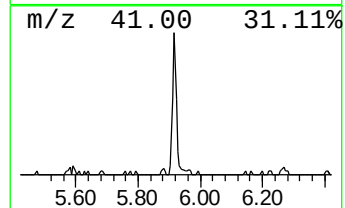
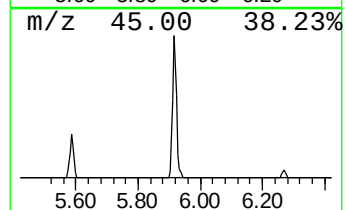
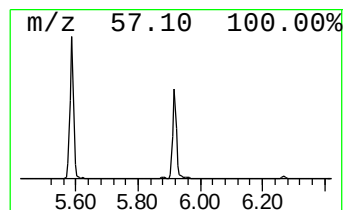
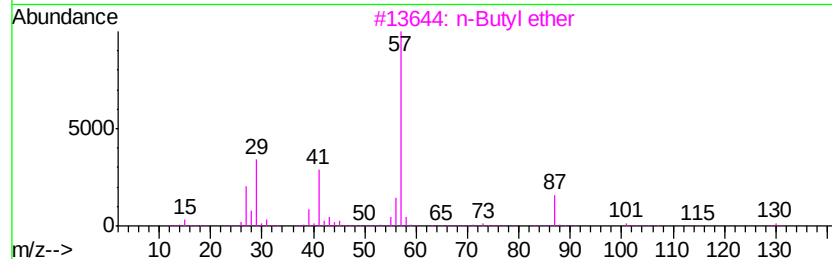
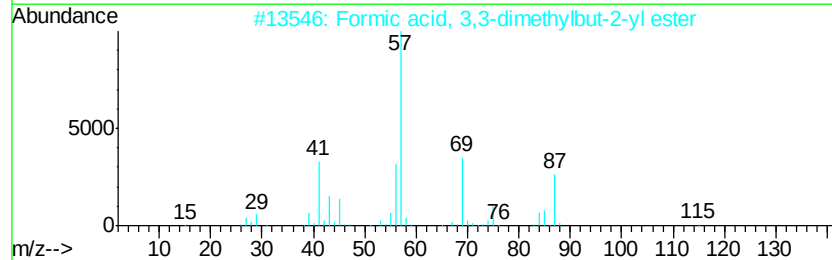
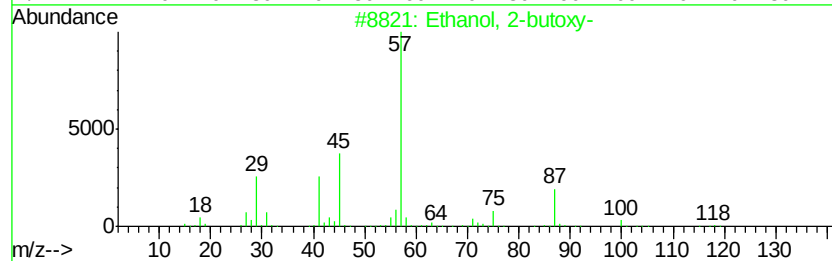
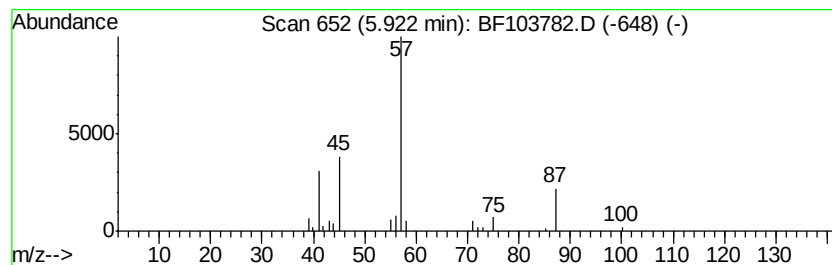
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Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.92	2.15 ng	82019	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	78
2		Formic acid, 3,3-dimethylbut-2-yl...	130	C7H14O2	1000368-20-5	64
3		n-Butyl ether	130	C8H18O	000142-96-1	37
4		1-Butene, 4-butoxy-	128	C8H16O	034061-76-2	25
5		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	23



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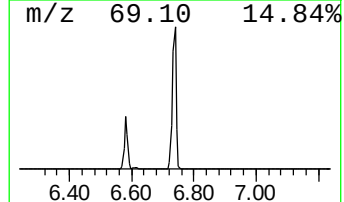
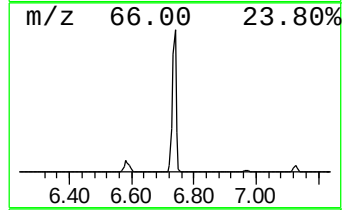
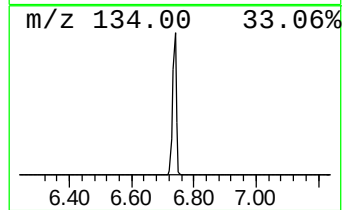
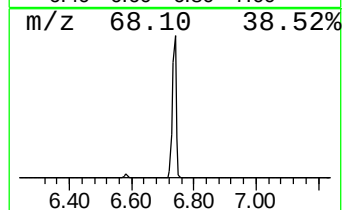
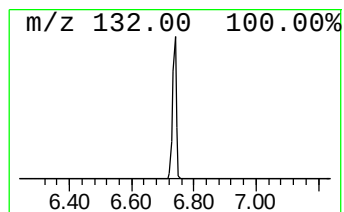
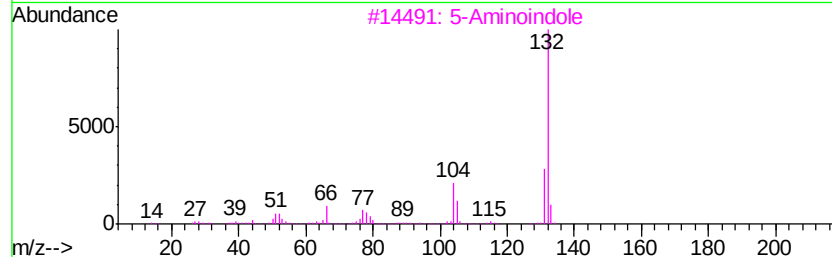
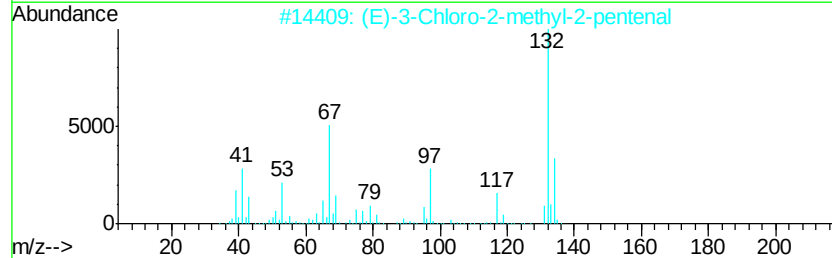
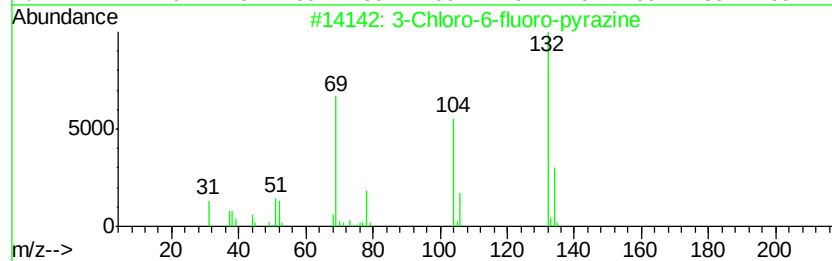
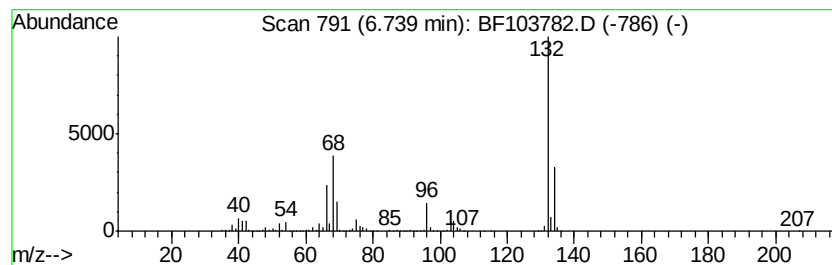
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Peak Number 4 unknown6.74 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	54.34 ng	2068890	1,4-Dichlorobenzene-d4	6.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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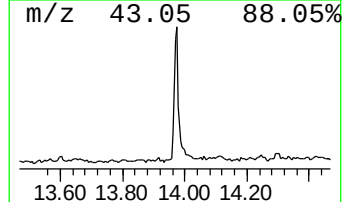
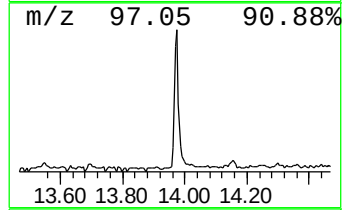
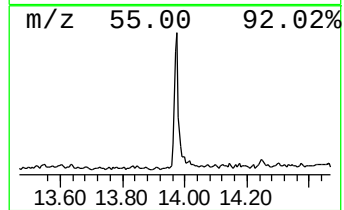
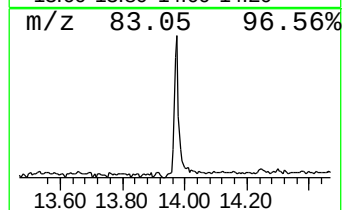
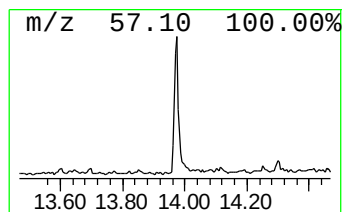
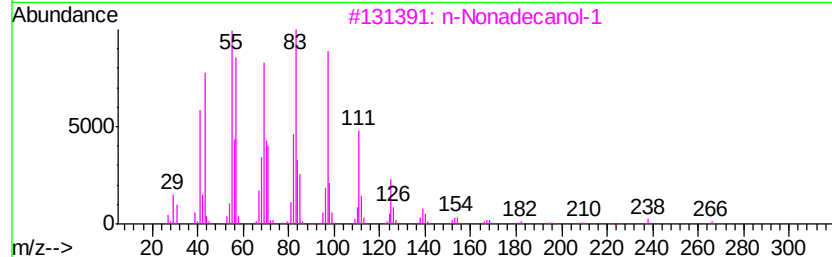
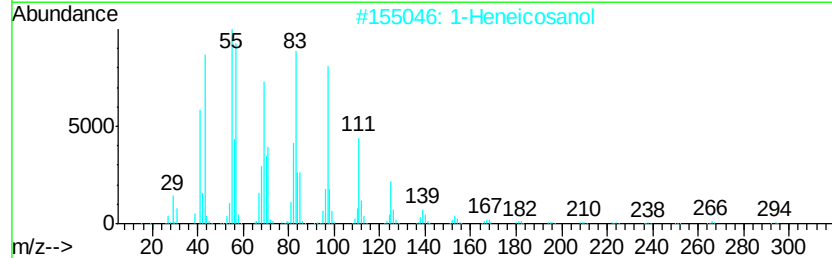
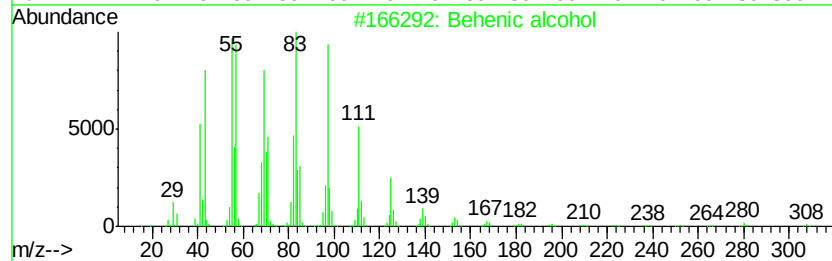
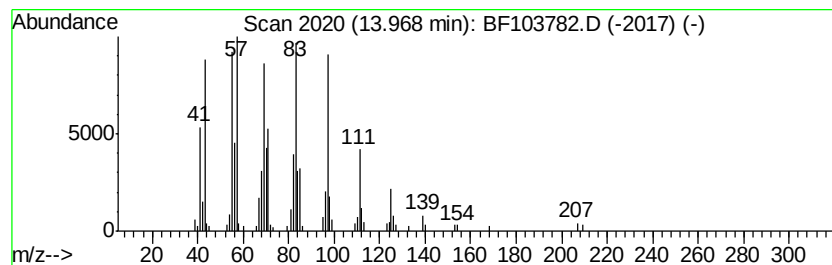
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.97	4.90 ng	185140	Chrysene-d12	14.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		n-Nonadecanol-1	284	C19H40O	001454-84-8	95
4		1-Heptacosanol	396	C27H56O	002004-39-9	94
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.30	12.9	ng	491172	1	6.97	761474	20.0
2-Pentanone, 4-hy...	5.20	2.6	ng	99086	1	6.97	761474	20.0
Ethanol, 2-butoxy-	5.92	2.1	ng	82019	1	6.97	761474	20.0
unknown6.74	6.74	54.3	ng	2068890	1	6.97	761474	20.0
Behenic alcohol	13.97	4.9	ng	185140	5	14.16	755907	20.0