

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF091521\
 Data File : BF125519.D
 Acq On : 15 Sep 2021 23:17
 Operator : JU/CG
 Sample : M3684-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 F006130

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:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF125519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.222	14	23	28	rVB	1452932	1926901	41.58%	6.172%
2	4.481	402	407	417	rVB	88399	110617	2.39%	0.354%
3	5.099	506	512	528	rVB	1507012	2119838	45.74%	6.790%
4	5.498	576	580	583	rBV	3404595	3329741	71.85%	10.666%
5	6.504	745	751	754	rBV	3110527	3447457	74.39%	11.043%
6	6.863	809	812	816	rBV	1211913	1016074	21.93%	3.255%
7	7.428	903	908	912	rBV	2066272	2354597	50.81%	7.542%
8	8.051	1011	1014	1026	rBV	91930	182006	3.93%	0.583%
9	8.145	1026	1030	1034	rVV	1277091	1331812	28.74%	4.266%
10	9.228	1208	1214	1217	rBV	4070473	4193299	90.49%	13.432%
11	9.904	1324	1329	1333	rBV	1687870	1552464	33.50%	4.973%
12	10.698	1460	1464	1478	rBV	721231	750308	16.19%	2.403%
13	11.398	1578	1583	1586	rBV	1796080	1635381	35.29%	5.239%
14	12.986	1848	1853	1856	rBV	4917746	4634107	100.00%	14.844%
15	13.904	2006	2009	2012	rBV	84251	86639	1.87%	0.278%
16	14.039	2028	2032	2036	rVB	1603205	1393860	30.08%	4.465%
17	15.527	2279	2285	2293	rVB	928788	1152945	24.88%	3.693%

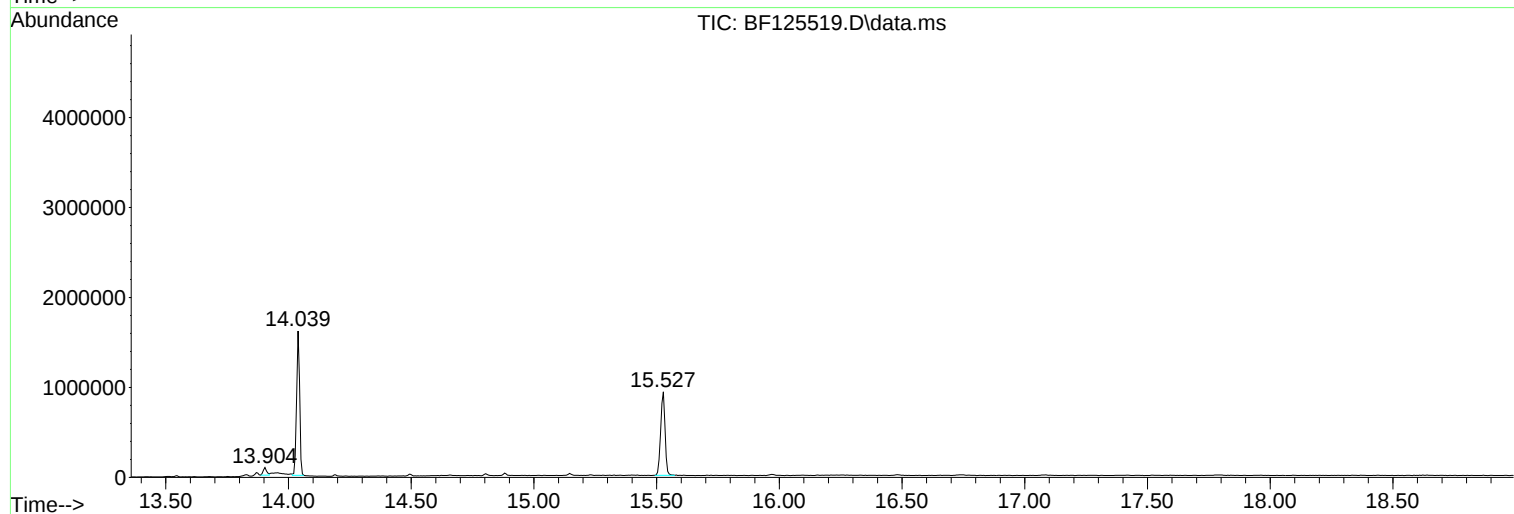
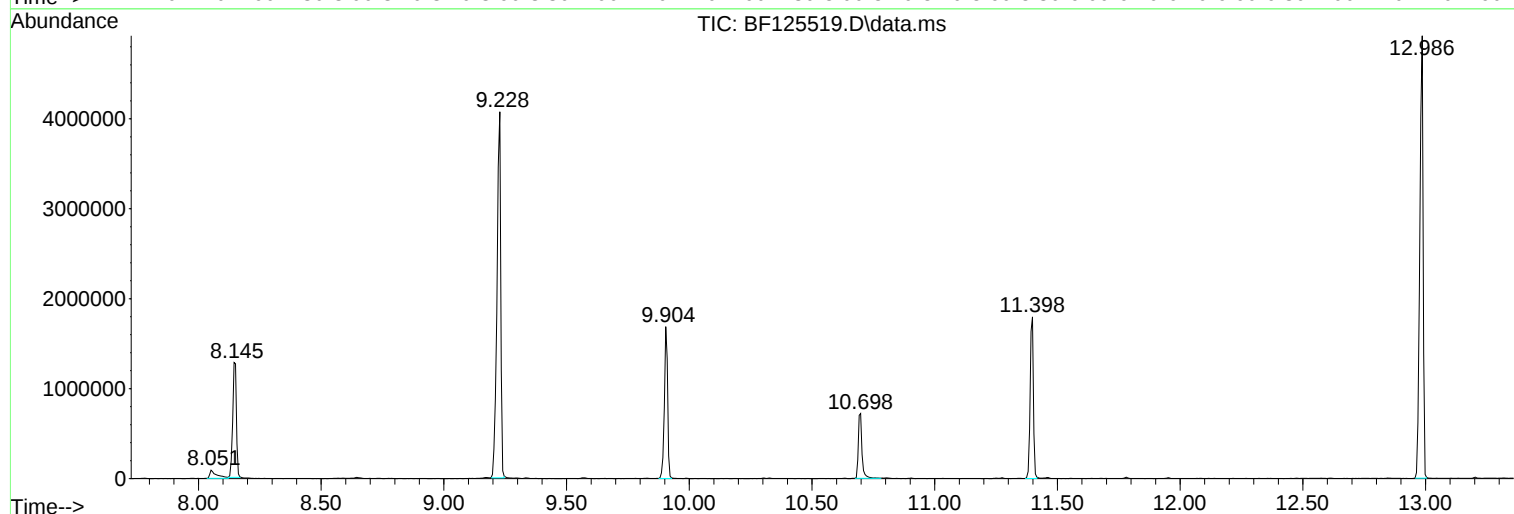
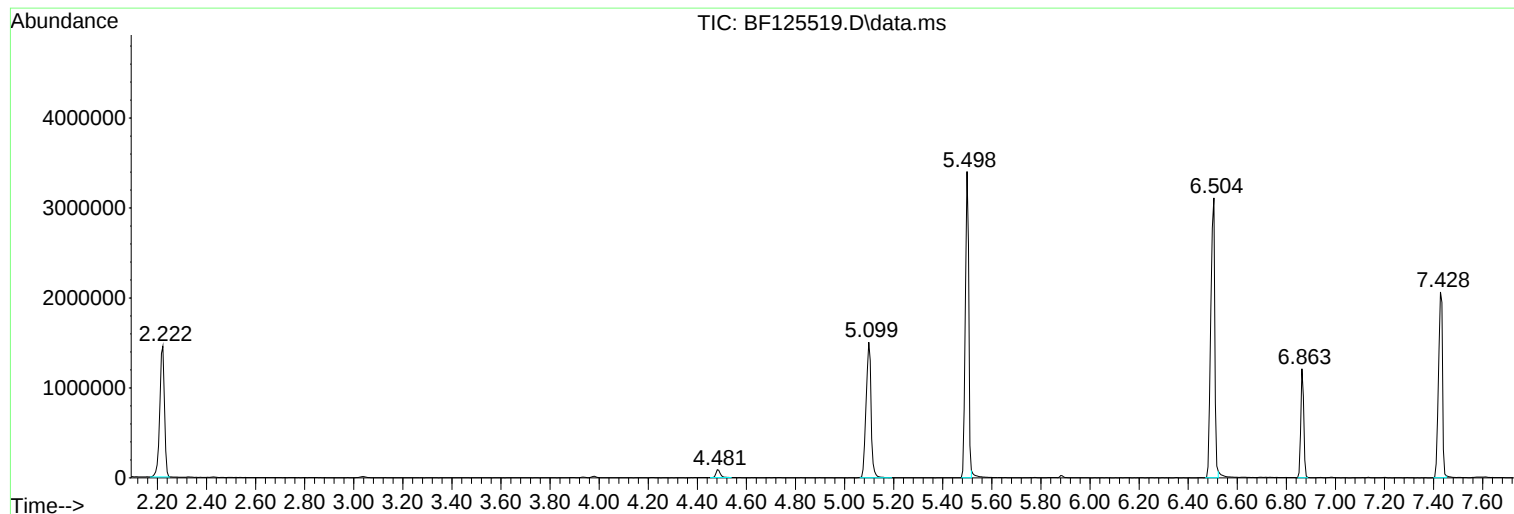
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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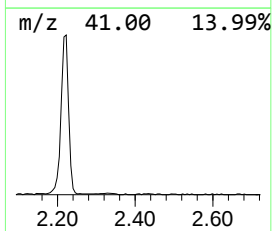
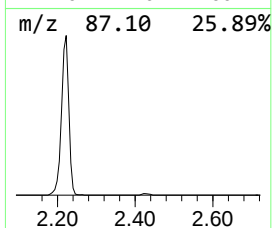
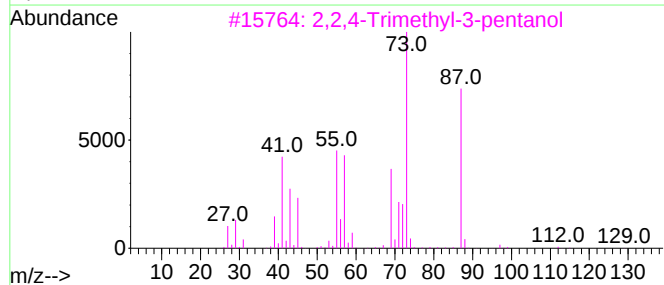
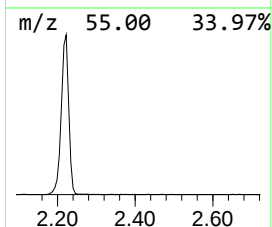
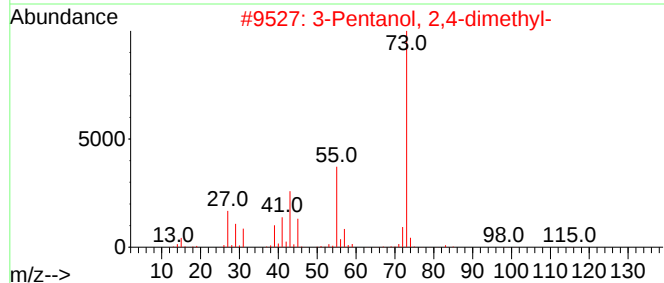
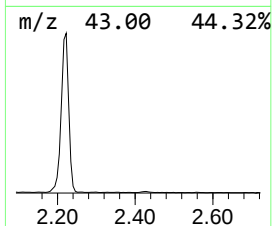
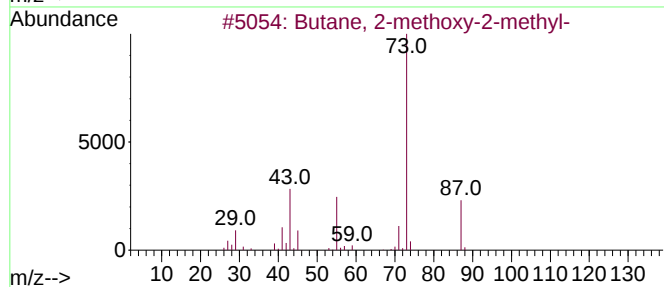
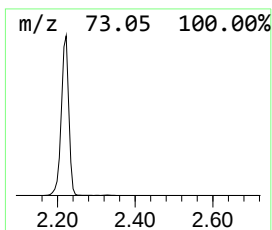
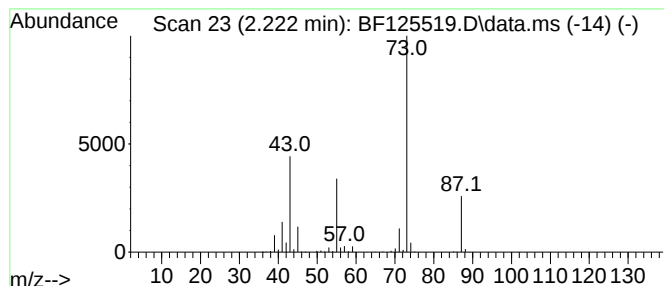
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF091521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.222	37.93 ng	1926900	1,4-Dichlorobenzene-d4	6.863

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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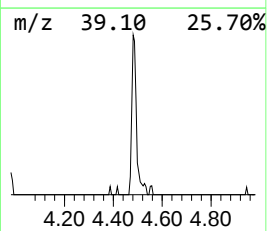
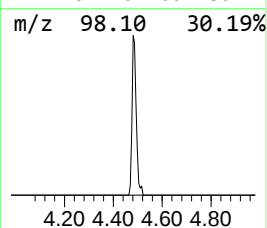
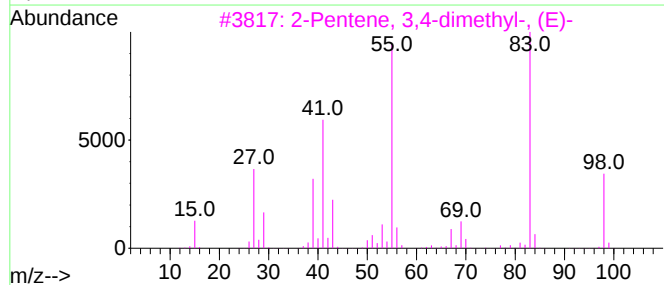
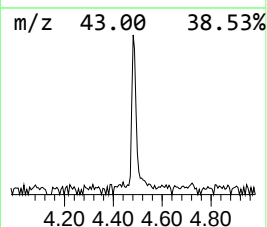
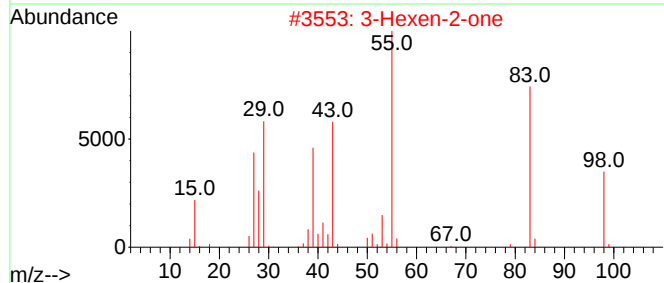
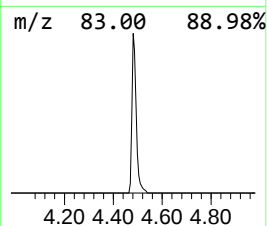
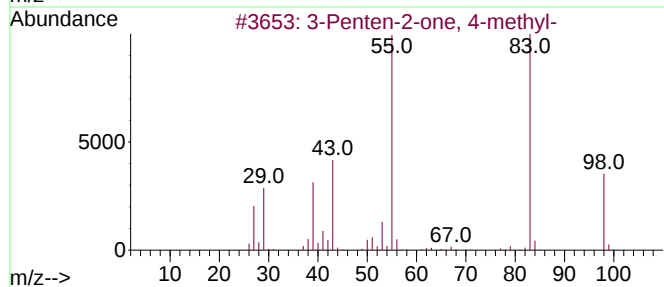
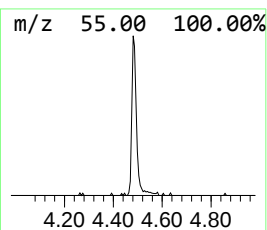
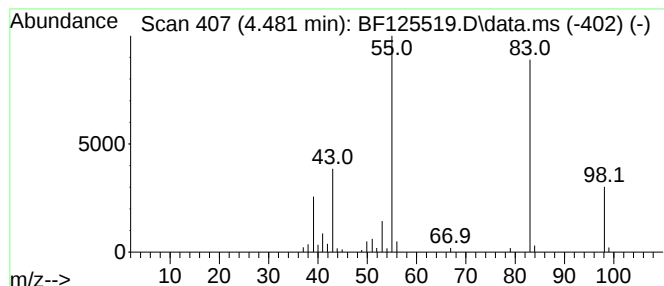
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.481	2.18 ng	110617	1,4-Dichlorobenzene-d4	6.863

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	90
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4		2-Pentene, 4,4-dimethyl-	98	C7H14	026232-98-4	78
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	78



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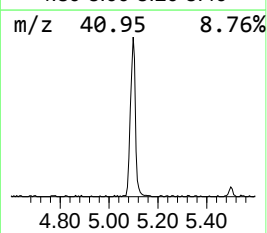
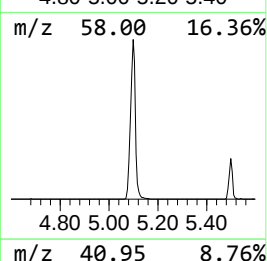
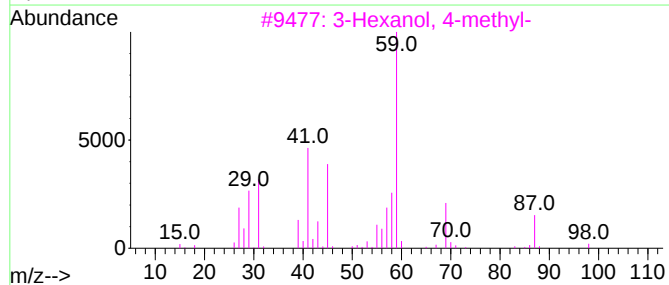
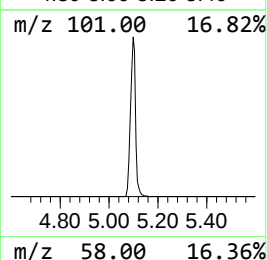
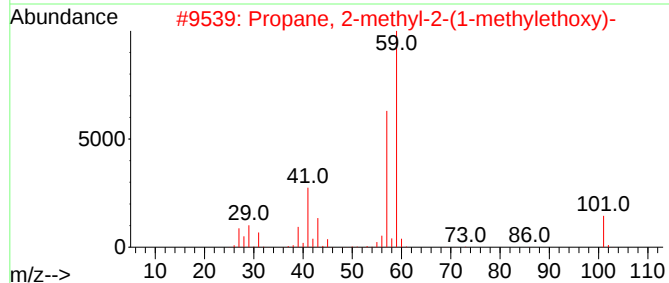
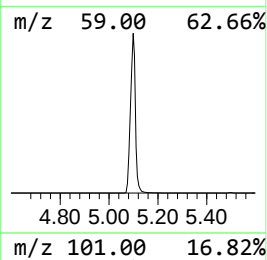
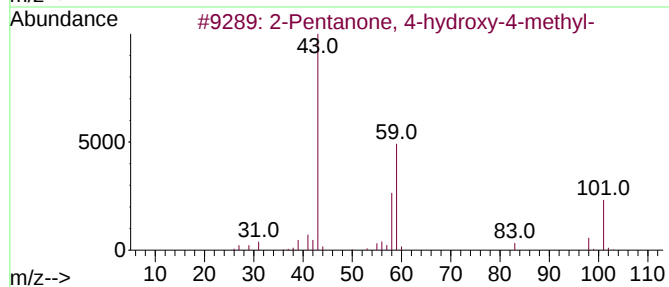
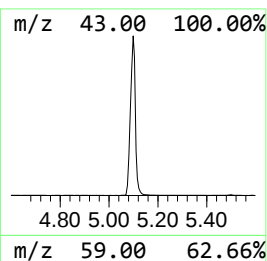
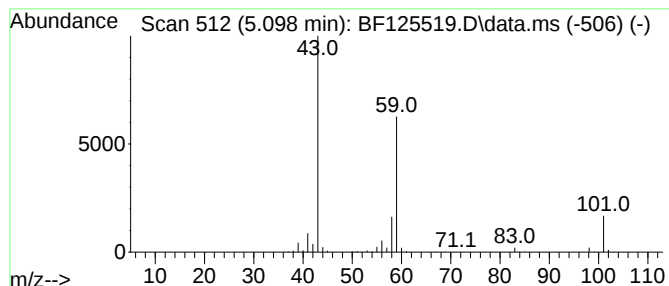
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.098	41.73 ng	2119840	1,4-Dichlorobenzene-d4	6.863	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23



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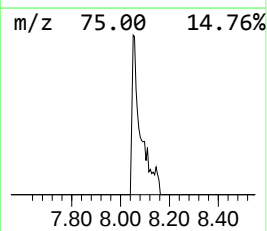
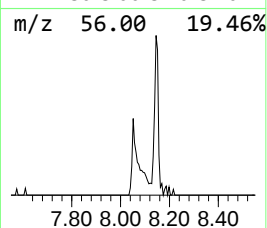
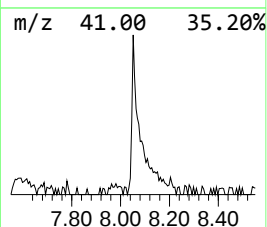
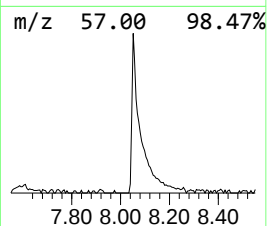
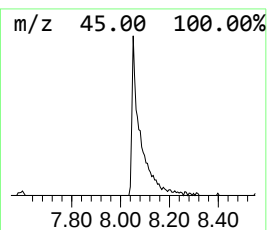
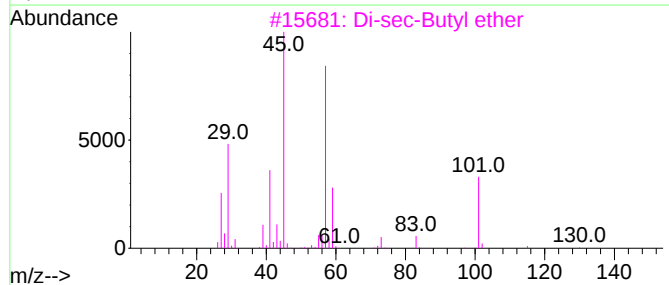
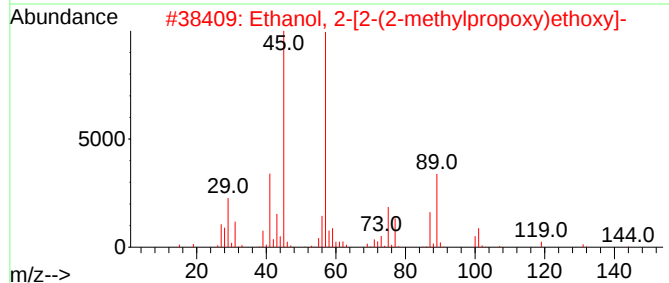
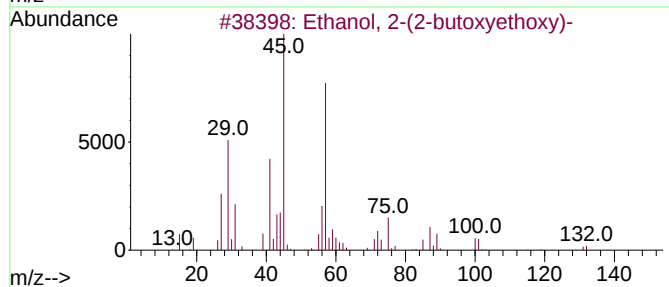
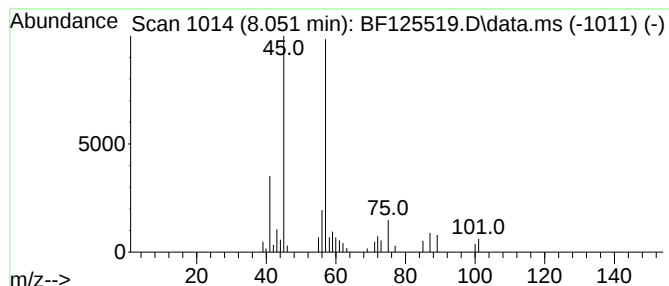
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.051	2.73 ng	182006	Naphthalene-d8	8.151

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
3			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50
4			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	50
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	47



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.222	37.9	ng	1926900	1	6.863	1016070	20.0
3-Penten-2-one,...	4.481	2.2	ng	110617	1	6.863	1016070	20.0
2-Pentanone, 4-...	5.098	41.7	ng	2119840	1	6.863	1016070	20.0
Ethanol, 2-(2-b...	8.051	2.7	ng	182006	2	8.151	1331810	20.0