

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG070621\
 Data File : BG049190.D
 Acq On : 6 Jul 2021 18:13
 Operator : CG/JU
 Sample : M2933-01
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 1

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_G\METHODS\8270-BG063021.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049190.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.137	9	17	25	rBV3	61600	174470	8.67%	1.553%
2	3.219	25	31	38	rVB	21345	49101	2.44%	0.437%
3	5.170	359	363	372	rVB	15537	25615	1.27%	0.228%
4	5.640	436	443	453	rBV	615433	1072171	53.31%	9.541%
5	7.244	707	716	732	rBV	636518	1179956	58.66%	10.500%
6	7.379	732	739	749	rVB	17332	35787	1.78%	0.318%
7	7.673	785	789	796	rBV	14916	29951	1.49%	0.267%
8	8.084	853	859	870	rVB	148931	259151	12.88%	2.306%
9	9.254	1049	1058	1071	rBV	389842	709059	35.25%	6.310%
10	10.681	1294	1301	1307	rBV4	9478	21378	1.06%	0.190%
11	10.905	1330	1339	1349	rBV	196472	359418	17.87%	3.198%
12	13.349	1747	1755	1763	rBV	942243	1492643	74.21%	13.282%
13	14.171	1888	1895	1901	rBV	106907	163066	8.11%	1.451%
14	14.730	1984	1990	1998	rVB	295554	465760	23.16%	4.145%
15	16.216	2237	2243	2261	rBV	706705	1220750	60.69%	10.863%
16	17.479	2451	2458	2465	rBV	340734	526472	26.17%	4.685%
17	18.355	2603	2607	2613	rBV5	31506	49917	2.48%	0.444%
18	20.082	2895	2901	2909	rBV	1476140	2011359	100.00%	17.898%
19	21.392	3119	3124	3135	rBV2	123665	243429	12.10%	2.166%
20	21.762	3181	3187	3196	rVB	333138	549334	27.31%	4.888%
21	21.909	3208	3212	3217	rBV7	19944	33552	1.67%	0.299%
22	25.070	3740	3750	3762	rVB2	185800	565539	28.12%	5.032%

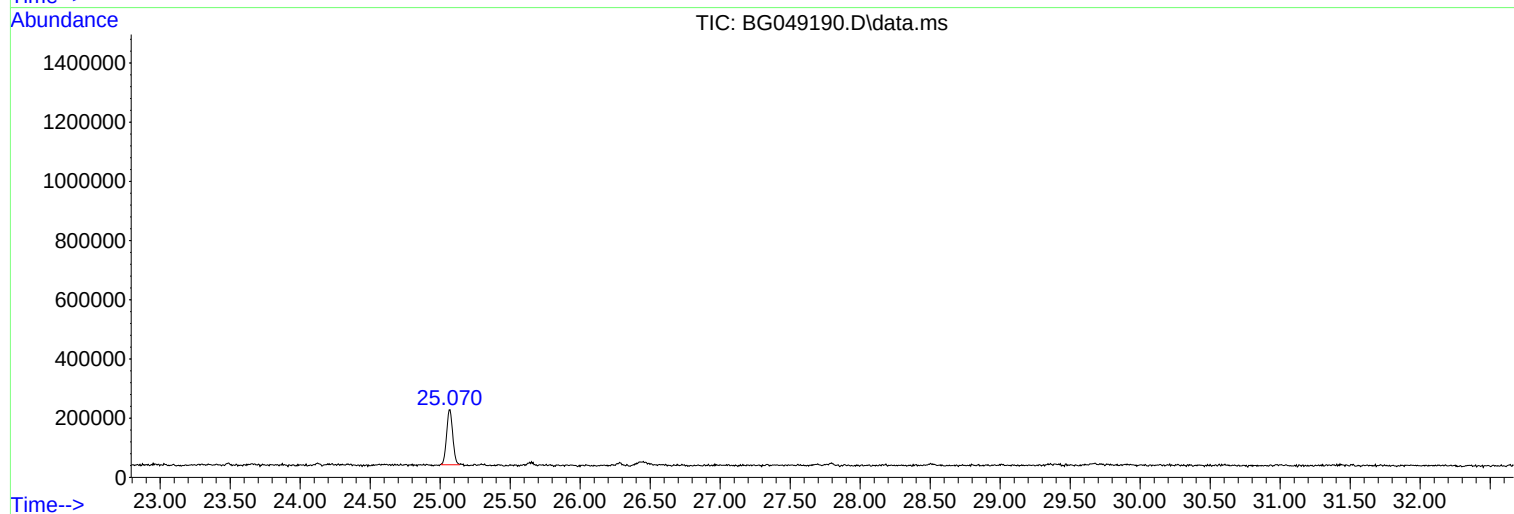
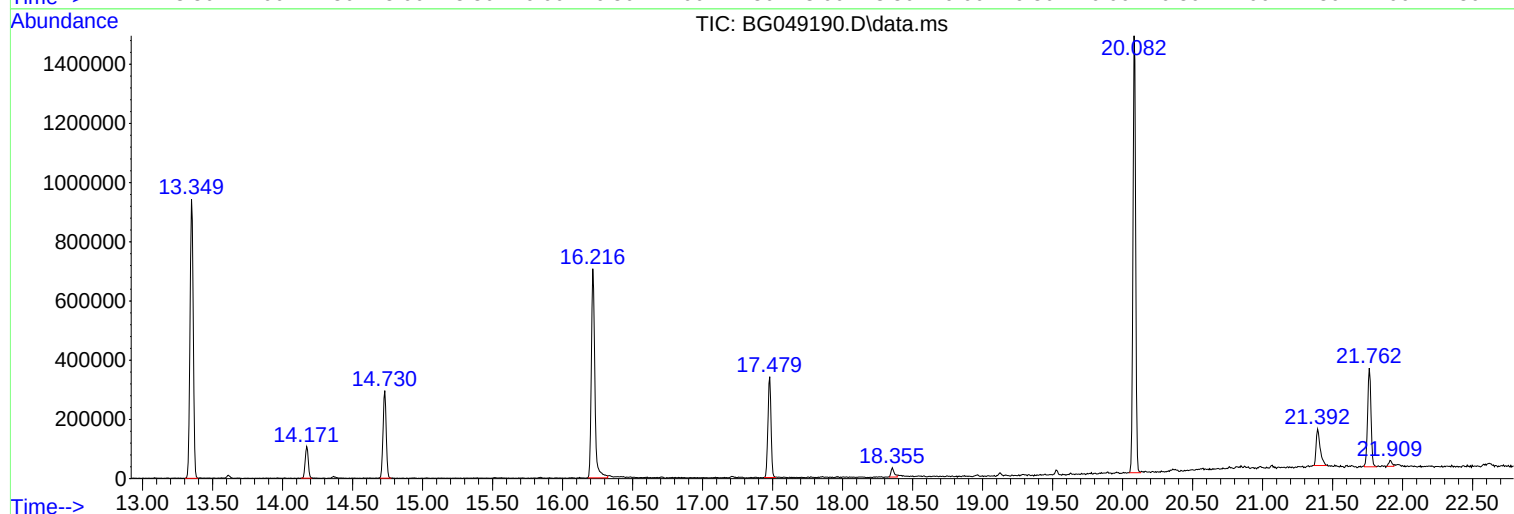
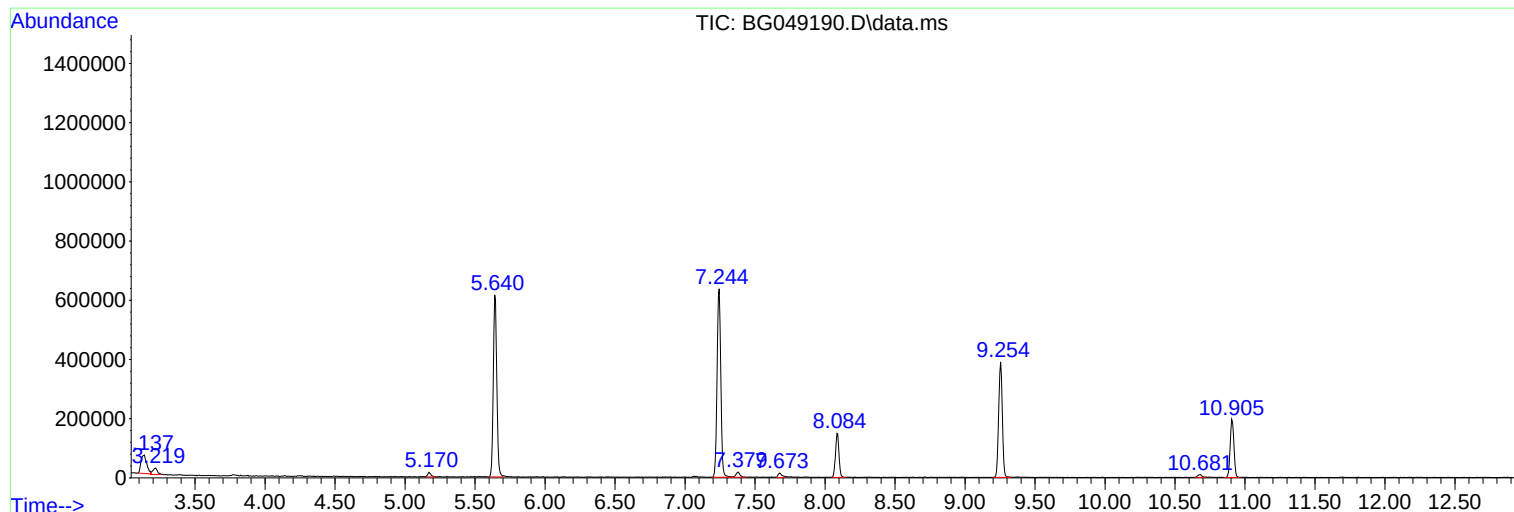
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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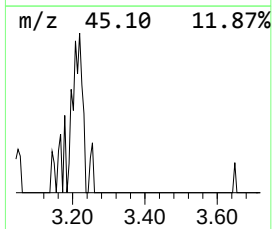
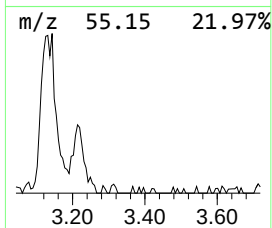
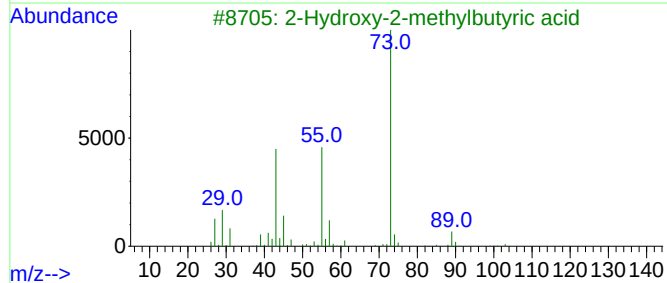
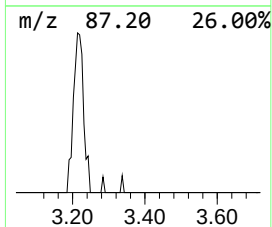
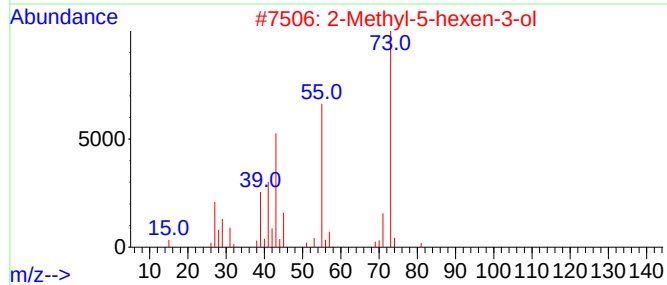
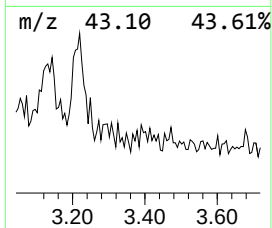
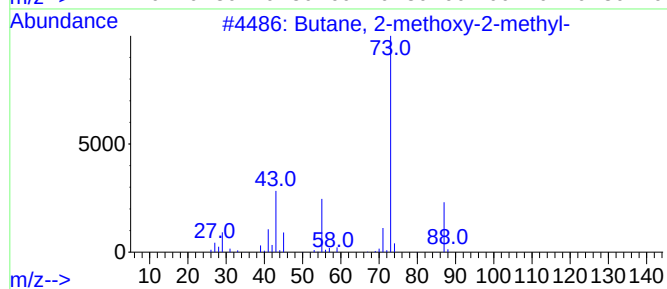
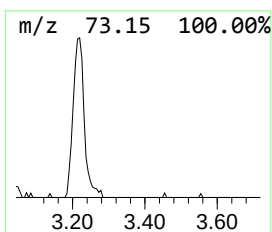
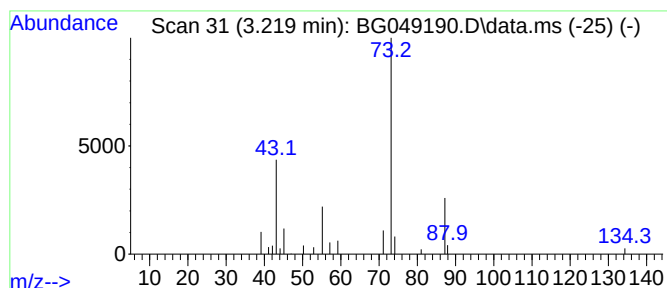
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.219	3.79 ng	49101	1,4-Dichlorobenzene-d4	8.090

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	37
3			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	12
4			1,3-Dioxolane, 2-(1-methylethyl)-	116	C6H12O2	000822-83-3	9
5			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	9



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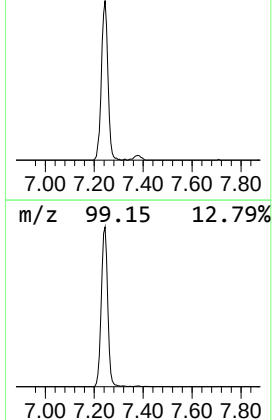
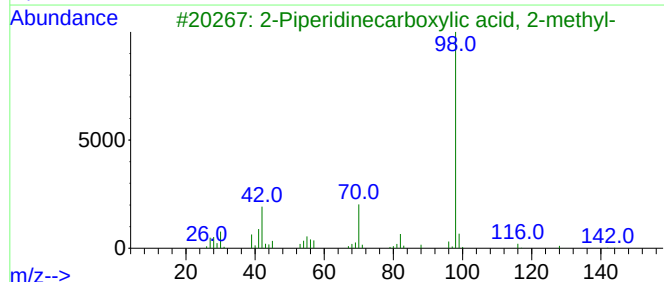
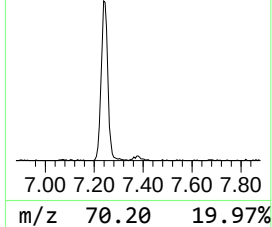
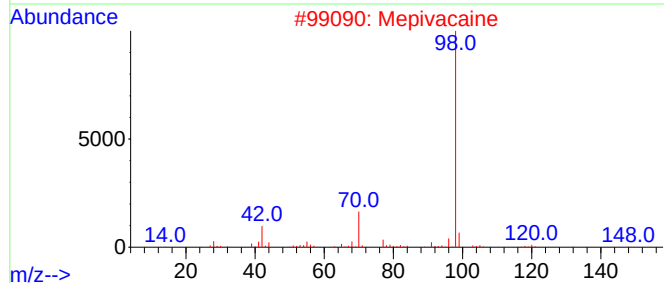
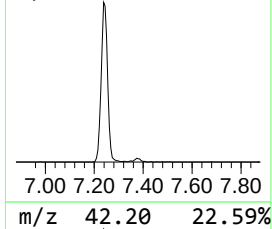
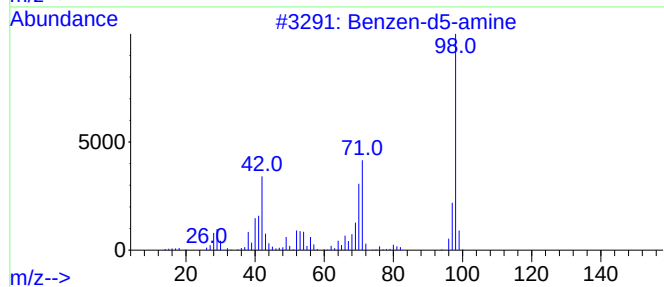
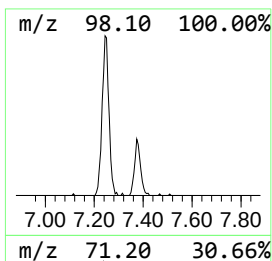
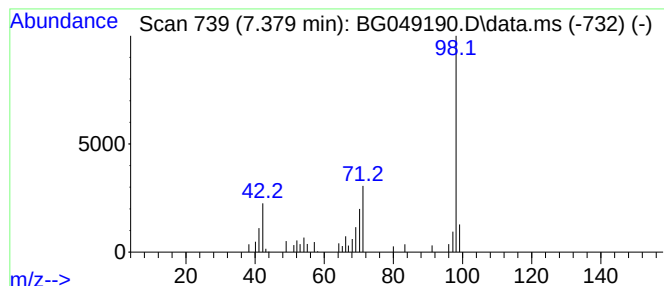
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG063021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Benzen-d5-amine Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.379	2.76 ng	35787	1,4-Dichlorobenzene-d4	8.090

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzen-d5-amine	98	C6H2D5N	004165-61-1	91
2			Mepivacaine	246	C15H22N2O	000096-88-8	53
3			2-Piperidinecarboxylic acid, 2-m...	143	C7H13NO2	072518-41-3	53
4			2,3-2H-4-Methyl-imidazole-2-one	98	C4H6N2O	039799-77-4	53
5			3H-Pyrazole, 3,4-diamino-	98	C3H6N4	1000288-40-0	43



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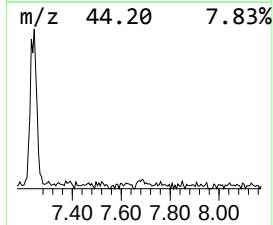
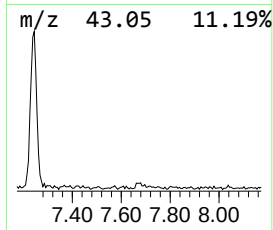
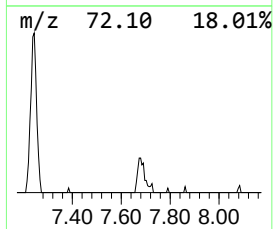
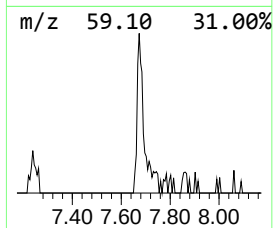
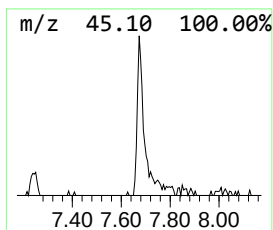
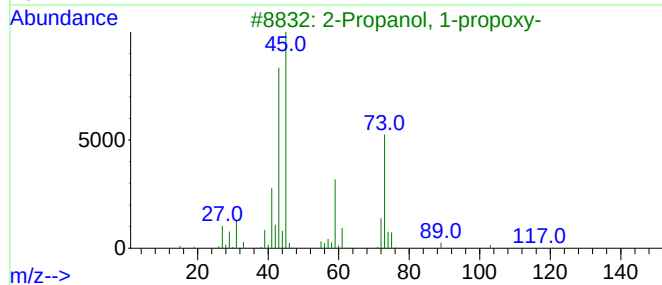
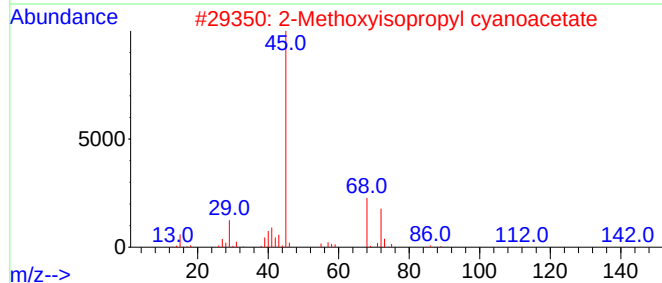
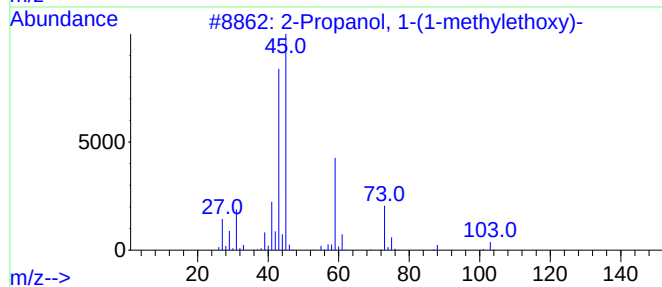
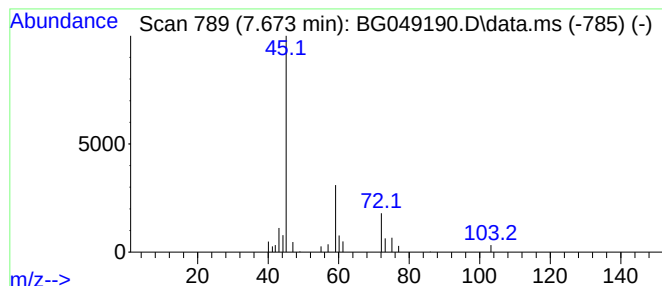
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.673 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.673	2.31 ng	29951	1,4-Dichlorobenzene-d4	8.090

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 1-(1-methylethoxy)-		118	C6H14O2	003944-36-3	39	
2	2-Methoxyisopropyl cyanoacetate		157	C7H11NO3	032804-79-8	36	
3	2-Propanol, 1-propoxy-		118	C6H14O2	001569-01-3	9	
4	Ethanol, 2-methoxy-, carbonate (...)		178	C7H14O5	000626-84-6	9	
5	Diethyl carbitol		162	C8H18O3	000112-36-7	9	



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Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
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ClientSampled :
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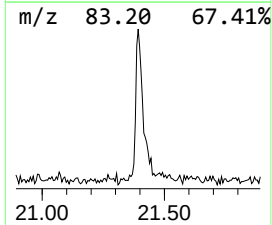
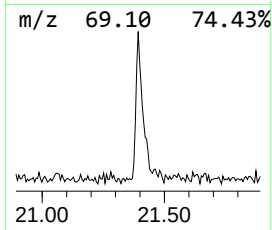
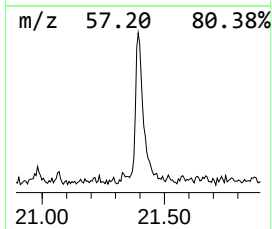
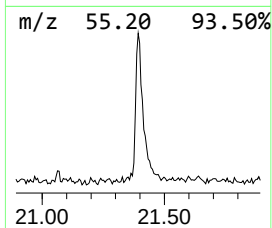
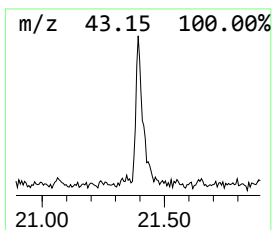
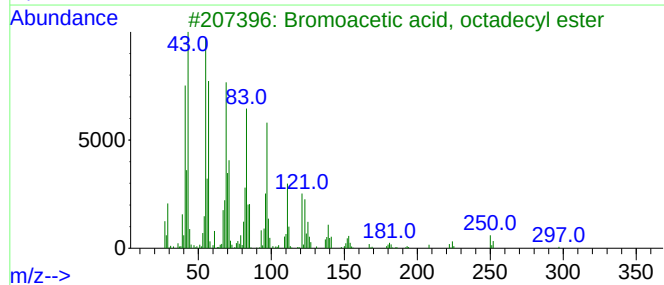
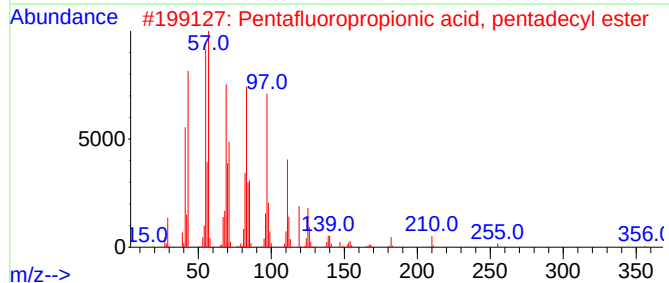
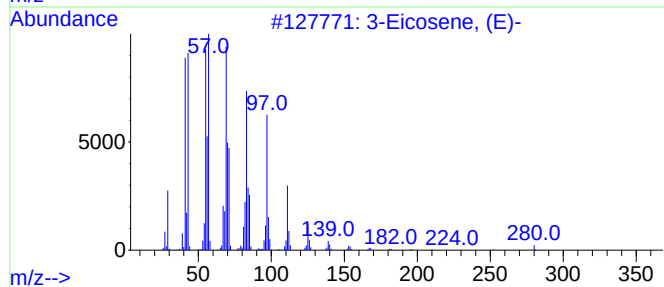
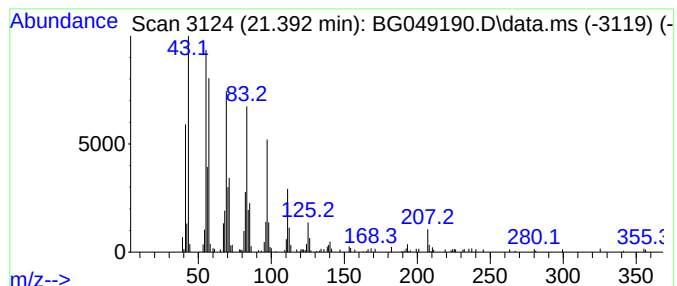
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Peak Number 5 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.392	8.86 ng	243429	Chrysene-d12	21.762

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Eicosene, (E)-	280	C20H40	074685-33-9	98
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
3			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	94
4			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
5			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.219	3.8	ng	49101	1	8.090	259151	20.0
Benzen-d5-amine	7.379	2.8	ng	35787	1	8.090	259151	20.0
unknown7.673	7.673	2.3	ng	29951	1	8.090	259151	20.0
3-Eicosene, (E)-	21.392	8.9	ng	243429	5	21.762	549334	20.0