

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG061821\
 Data File : BG049026.D
 Acq On : 18 Jun 2021 19:16
 Operator : CG/JU
 Sample : M2709-03
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 0236-COMPOSITE-M

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-BG061121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG049026.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.156	15	20	30	rBV	114141	261850	12.21%	2.691%
2	3.238	31	34	39	rVB3	21915	30788	1.44%	0.316%
3	5.195	361	367	375	rBV2	37148	64410	3.00%	0.662%
4	5.665	440	447	462	rVB	488677	808698	37.71%	8.310%
5	7.263	712	719	728	rBV	492065	861444	40.16%	8.852%
6	8.109	856	863	870	rBV2	123230	218538	10.19%	2.246%
7	9.278	1052	1062	1071	rBV	288157	521802	24.33%	5.362%
8	10.700	1297	1304	1313	rBV3	15368	29725	1.39%	0.305%
9	10.935	1337	1344	1354	rVB	157249	292859	13.65%	3.009%
10	13.373	1750	1759	1768	rVB	678640	1056942	49.28%	10.861%
11	14.754	1985	1994	2001	rBV	251187	402815	18.78%	4.139%
12	16.240	2239	2247	2256	rBV	692171	1097112	51.15%	11.274%
13	17.504	2455	2462	2468	rBV	333512	535350	24.96%	5.501%
14	20.106	2899	2905	2911	rBV	1592414	2144764	100.00%	22.040%
15	21.423	3124	3129	3137	rBV4	50647	93577	4.36%	0.962%
16	21.787	3182	3191	3199	rBV2	370022	639772	29.83%	6.574%
17	23.314	3446	3451	3456	rBV5	21463	40383	1.88%	0.415%
18	25.118	3748	3758	3769	rBV2	216732	630601	29.40%	6.480%

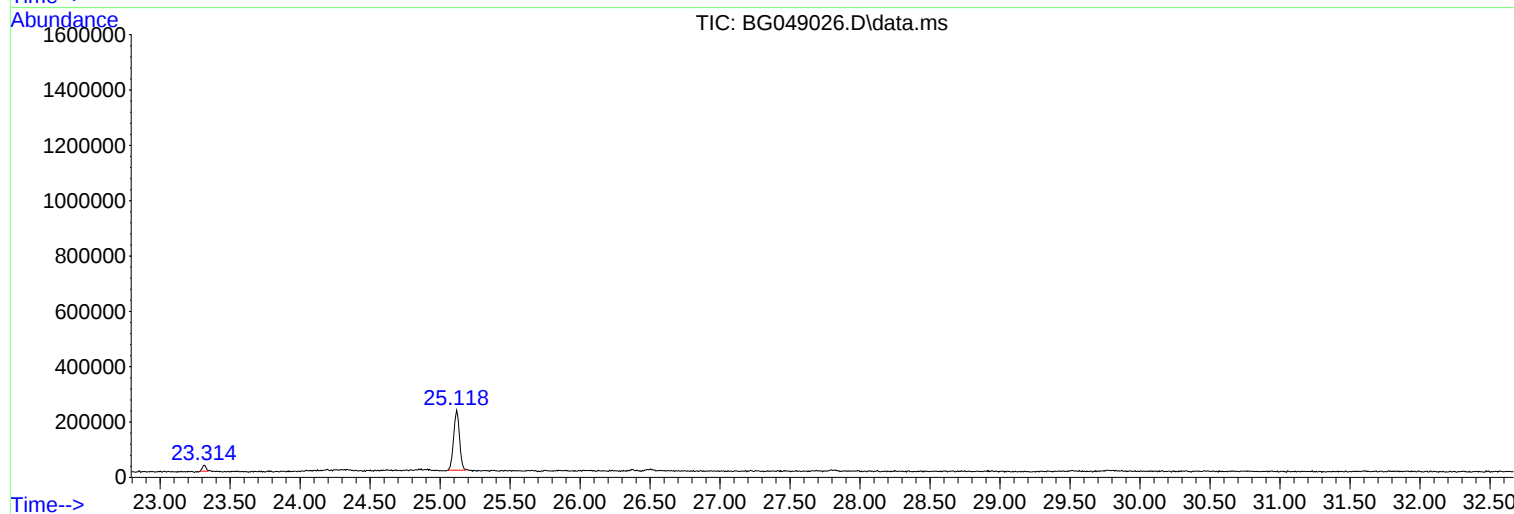
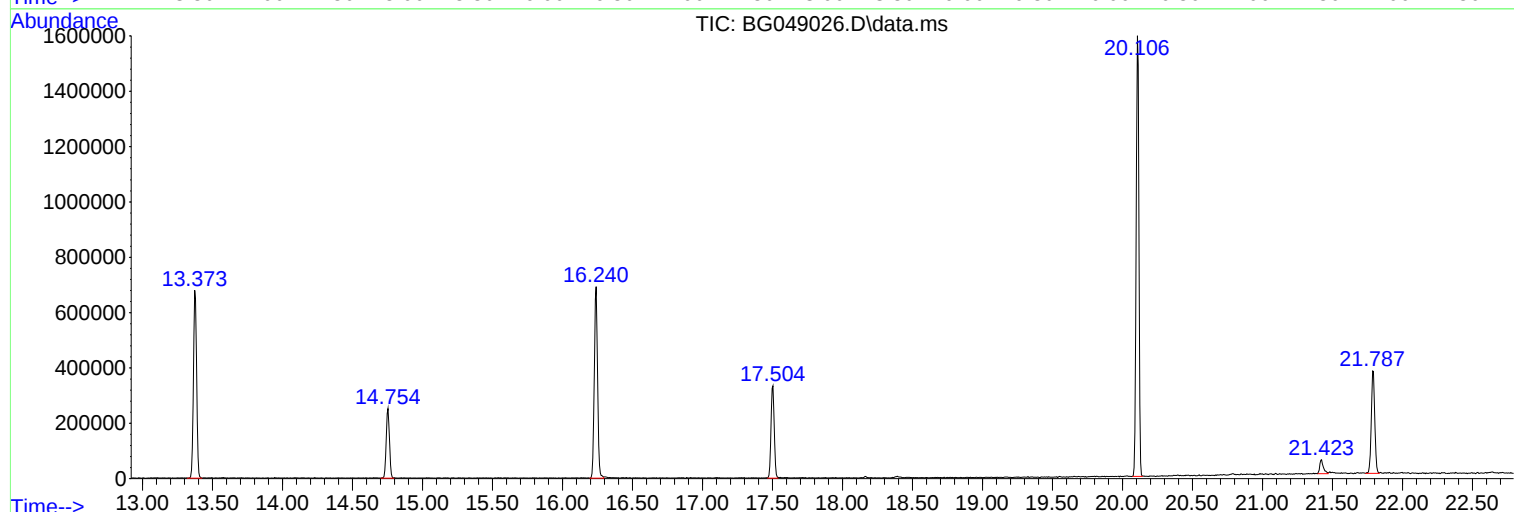
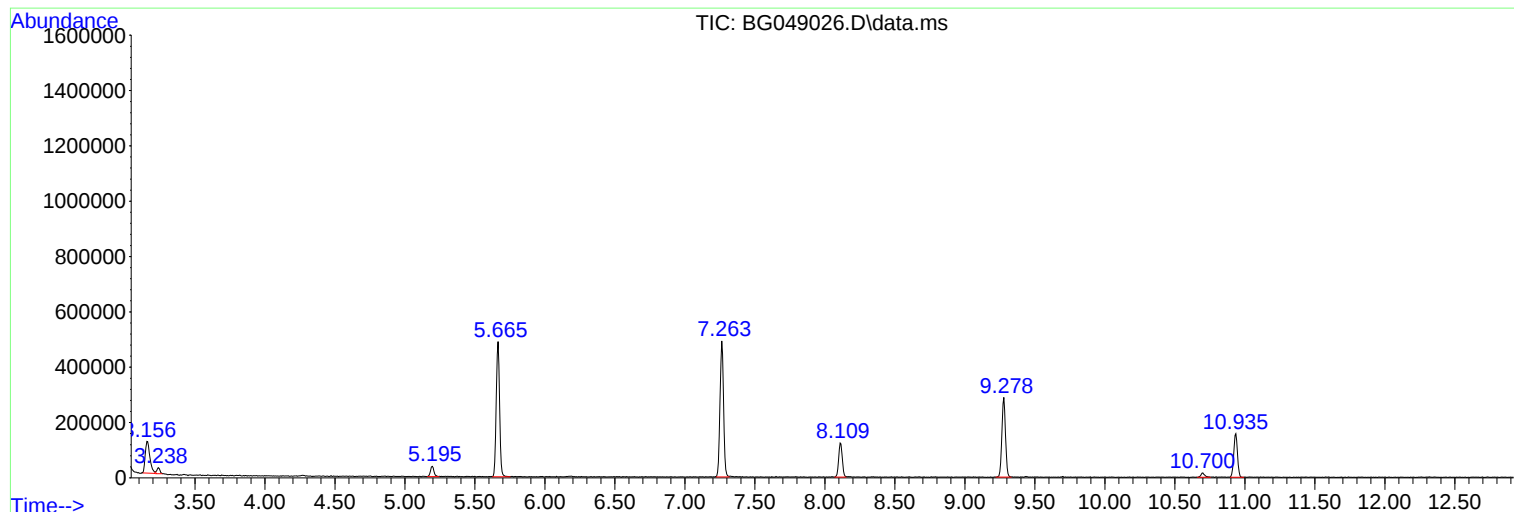
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ClientSampleId :
0236-COMPOSITE-M

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.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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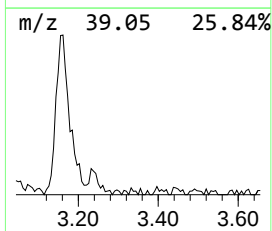
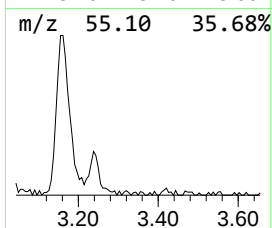
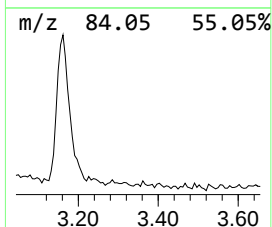
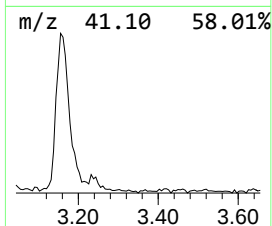
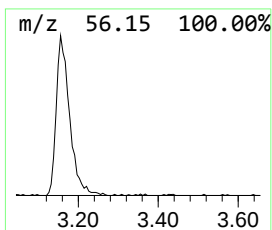
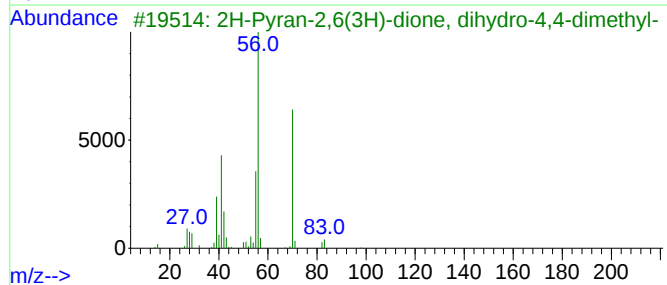
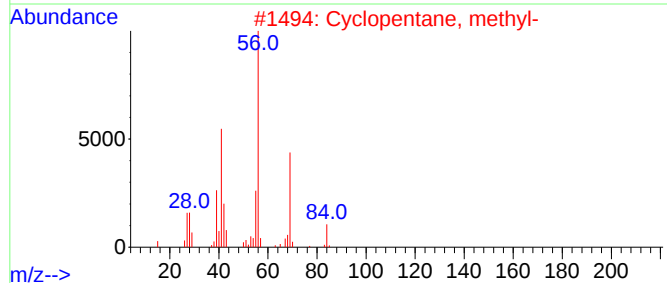
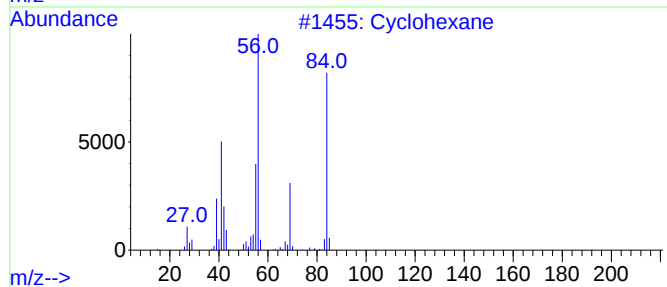
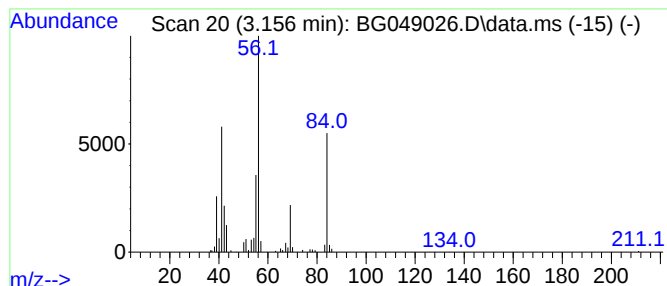
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG061121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Cyclohexane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.156	23.96 ng	261850	1,4-Dichlorobenzene-d4	8.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane	84	C6H12	000110-82-7	94
2			Cyclopentane, methyl-	84	C6H12	000096-37-7	53
3			2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	50
4			Cyanic acid, 2-methylpropyl ester	99	C5H9NO	001768-25-8	50
5			Cyclobutane	56	C4H8	000287-23-0	43



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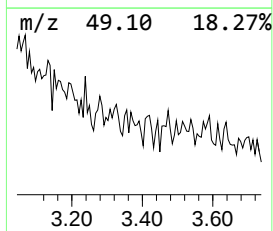
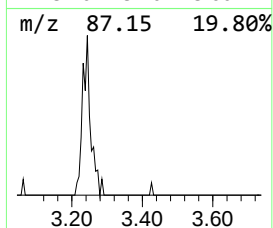
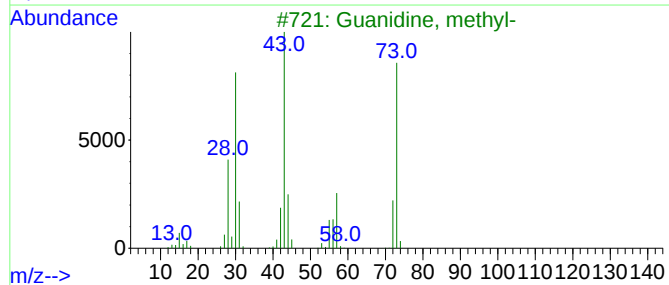
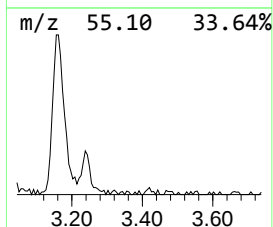
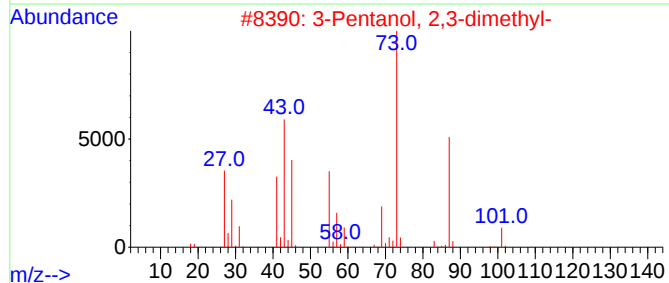
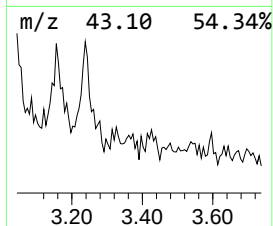
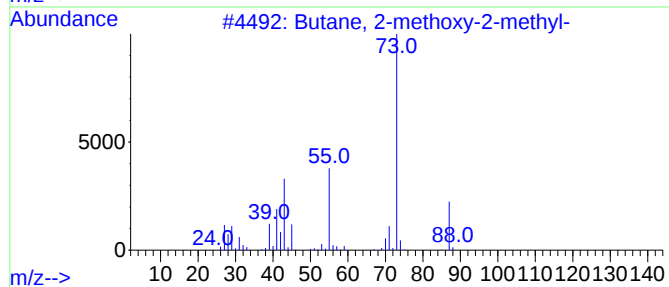
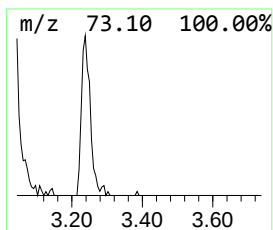
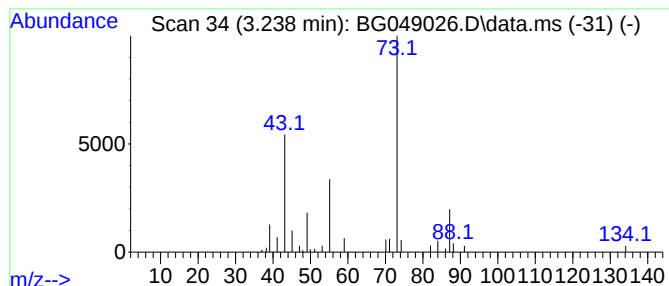
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TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown3.238 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.238	2.82 ng	30788	1,4-Dichlorobenzene-d4	8.109

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	33
2			3-Pentanol, 2,3-dimethyl-	116	C7H16O	000595-41-5	10
3			Guanidine, methyl-	73	C2H7N3	000471-29-4	9
4			Propenoic acid, 2-trifluoroacety...	183	C5H4F3NO3	000675-00-3	9
5			2-Methylbutane-1,4-diol, 3-(1-et...	192	C9H20O4	088481-54-3	9



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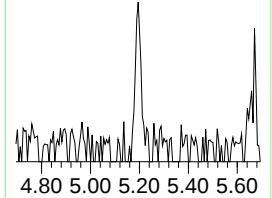
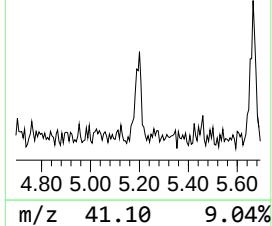
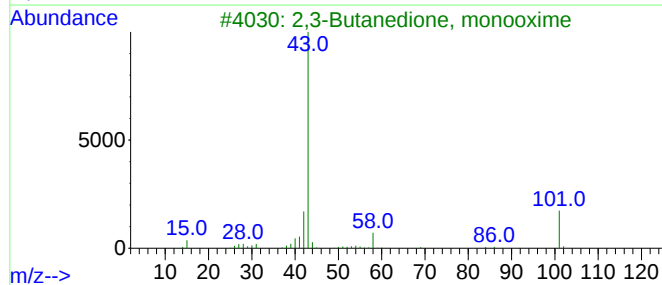
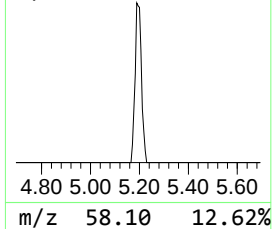
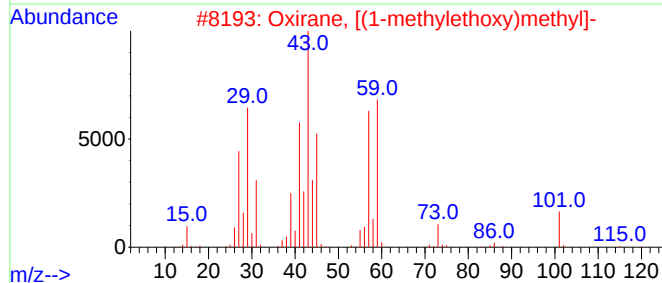
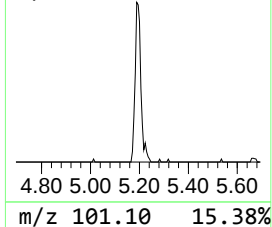
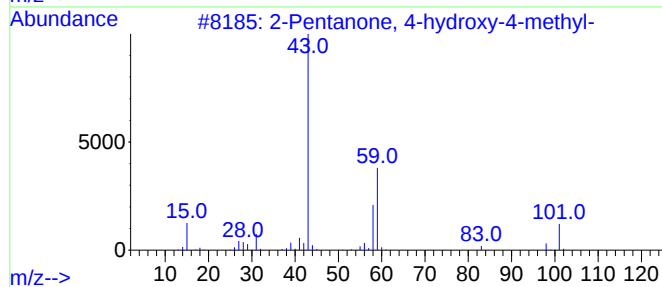
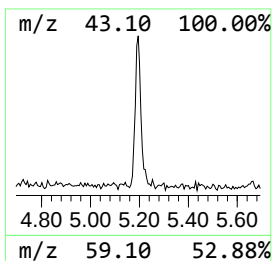
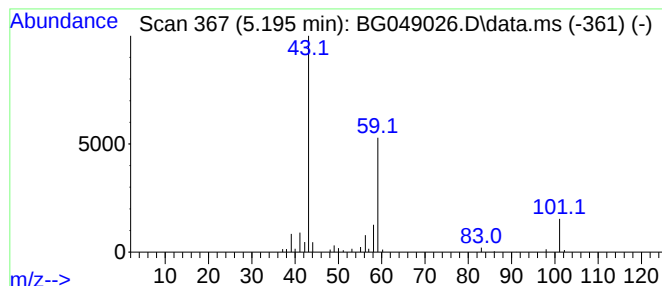
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.195	5.89 ng	64410	1,4-Dichlorobenzene-d4	8.109

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Oxirane, [(1-methylethoxy)methyl]-	116	C6H12O2	004016-14-2	40
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	35
4		4-Penten-2-one, 4-methyl-	98	C6H10O	003744-02-3	9
5		Pentanal, oxime	101	C5H11NO	000628-79-5	9



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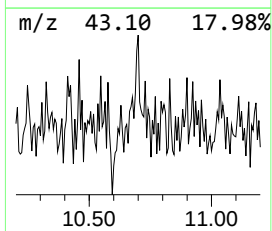
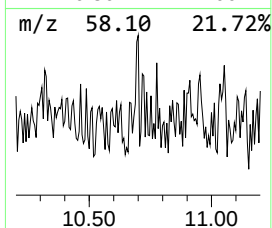
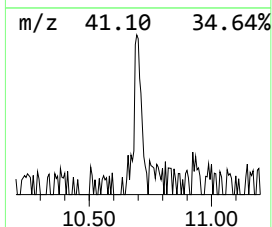
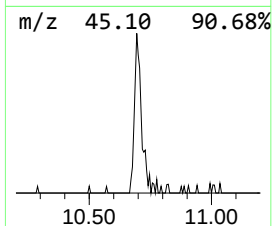
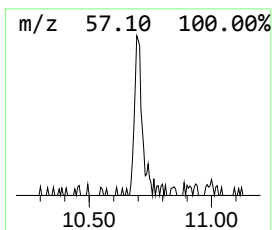
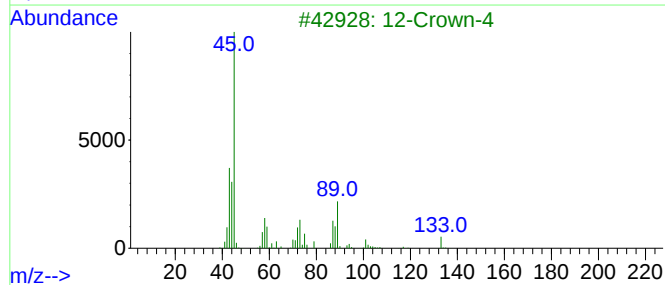
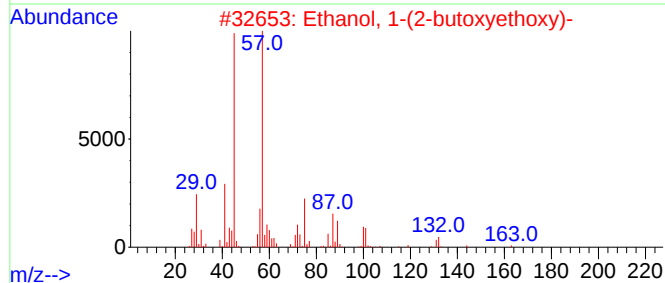
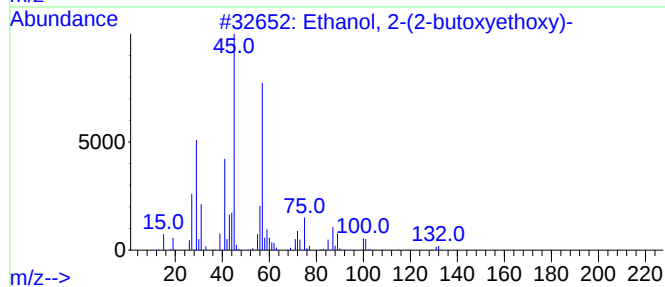
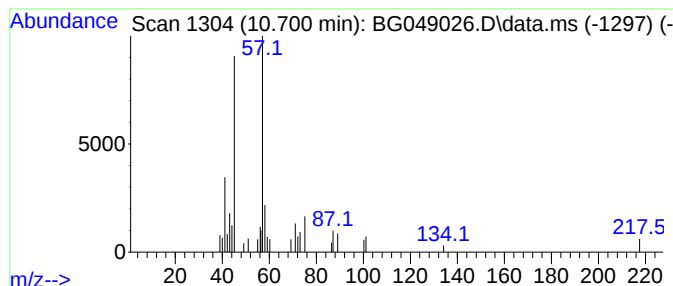
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Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.700	2.03 ng	29725	Naphthalene-d8	10.935

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	53
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	50
3			12-Crown-4	176	C8H16O4	000294-93-9	47
4			2-Propanol, 1-(2-butoxyethoxy)-	176	C9H20O3	000124-16-3	45
5			3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	45



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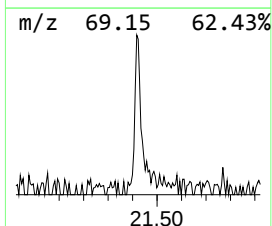
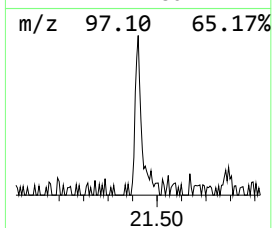
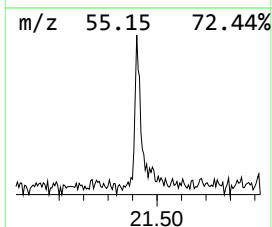
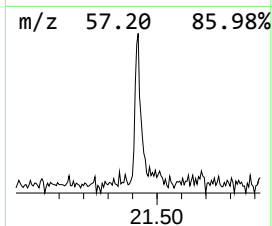
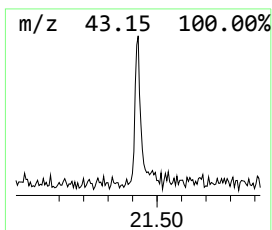
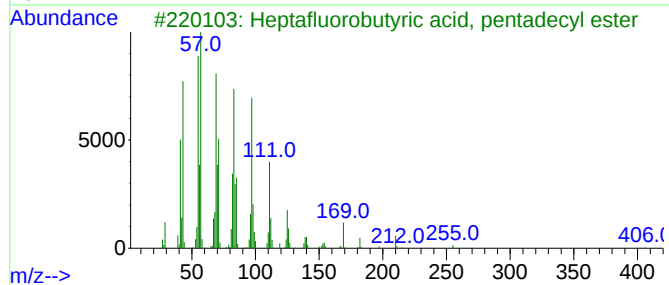
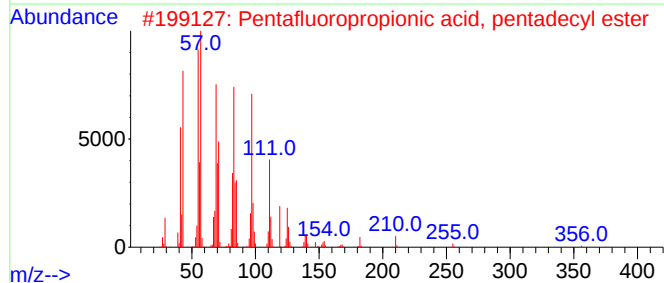
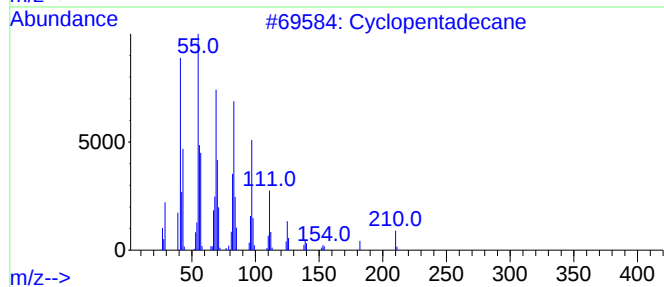
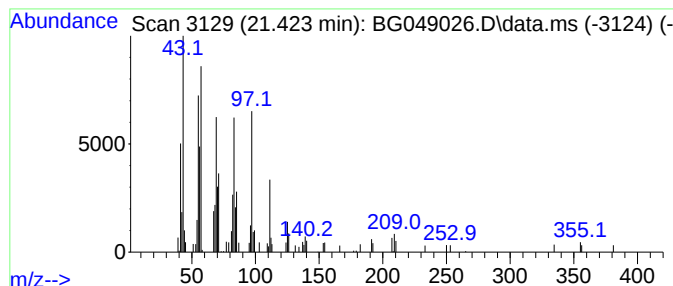
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Peak Number 5 Cyclopentadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.423	2.93 ng	93577	Chrysene-d12	21.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentadecane	210	C15H30	000295-48-7	91
2			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	90
4			1-Docosene	308	C22H44	001599-67-3	83
5			Heneicosyl heptafluorobutyrate	508	C25H43F7O2	1000351-83-8	76



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexane	3.156	24.0	ng	261850	1	8.109	218538	20.0
unknown3.238	3.238	2.8	ng	30788	1	8.109	218538	20.0
2-Pentanone, 4-...	5.195	5.9	ng	64410	1	8.109	218538	20.0
Ethanol, 2-(2-b...	10.700	2.0	ng	29725	2	10.935	292859	20.0
Cyclopentadecane	21.423	2.9	ng	93577	5	21.787	639772	20.0