

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG091222\
 Data File : BG054918.D
 Acq On : 12 Sep 2022 23:07
 Operator : CG/JU
 Sample : N4538-07
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MBD-SB-1-2-0-5

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-BG082522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG054918.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.202	320	326	333	rBV	33194	53703	2.44%	0.493%
2	5.684	400	408	420	rBV	610347	1025312	46.54%	9.412%
3	7.300	674	683	699	rBV	625988	1111930	50.47%	10.207%
4	8.140	820	826	836	rBV	157045	267402	12.14%	2.455%
5	9.315	1017	1026	1040	rBV	368320	690604	31.34%	6.339%
6	10.720	1258	1265	1276	rBV	18893	41969	1.90%	0.385%
7	10.966	1300	1307	1316	rBV	209387	385110	17.48%	3.535%
8	13.399	1714	1721	1733	rVB	1132519	1773358	80.49%	16.279%
9	13.651	1756	1764	1772	rBV	38973	62044	2.82%	0.570%
10	14.779	1944	1956	1964	rBV	326615	534930	24.28%	4.910%
11	16.266	2202	2209	2228	rBV	690488	1142919	51.87%	10.492%
12	17.523	2416	2423	2428	rBV	376838	604186	27.42%	5.546%
13	17.564	2428	2430	2437	rVB	32093	47216	2.14%	0.433%
14	18.158	2528	2531	2538	rBV2	18811	31069	1.41%	0.285%
15	19.327	2726	2730	2734	rVB2	60208	72660	3.30%	0.667%
16	19.456	2749	2752	2756	rBV	27546	34034	1.54%	0.312%
17	19.574	2768	2772	2777	rBV	73676	109074	4.95%	1.001%
18	19.938	2830	2834	2841	rVB	80379	124507	5.65%	1.143%
19	20.120	2860	2865	2871	rBV	1595368	2203273	100.00%	20.225%
20	21.818	3149	3154	3160	rVB2	345540	578428	26.25%	5.310%

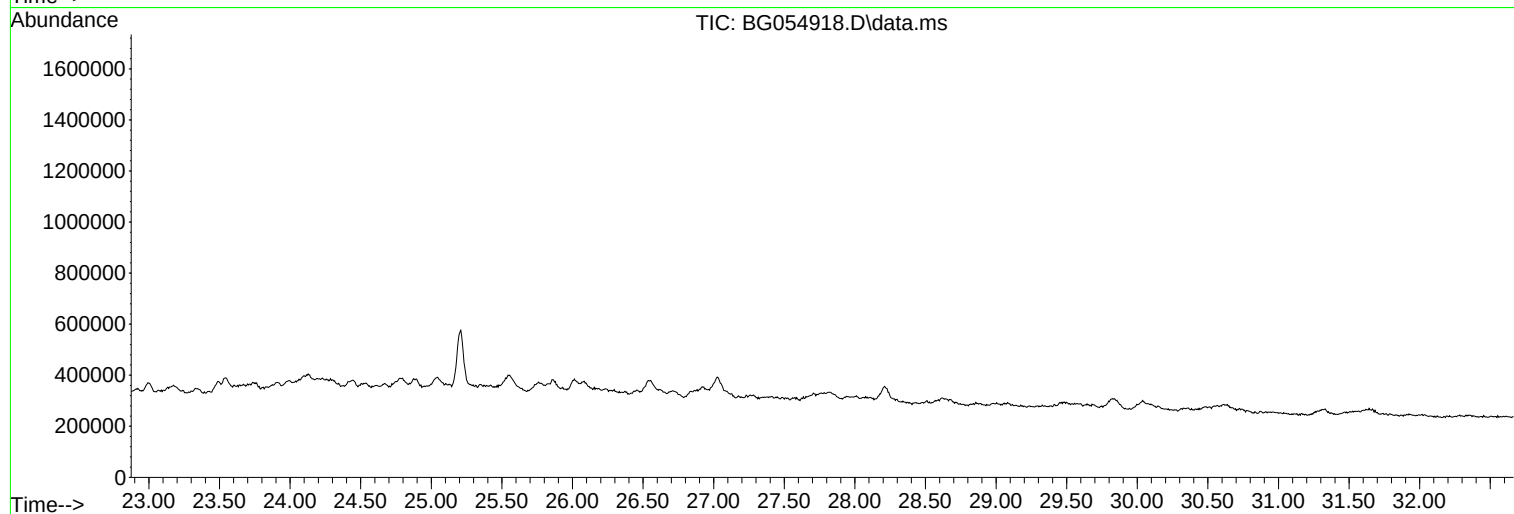
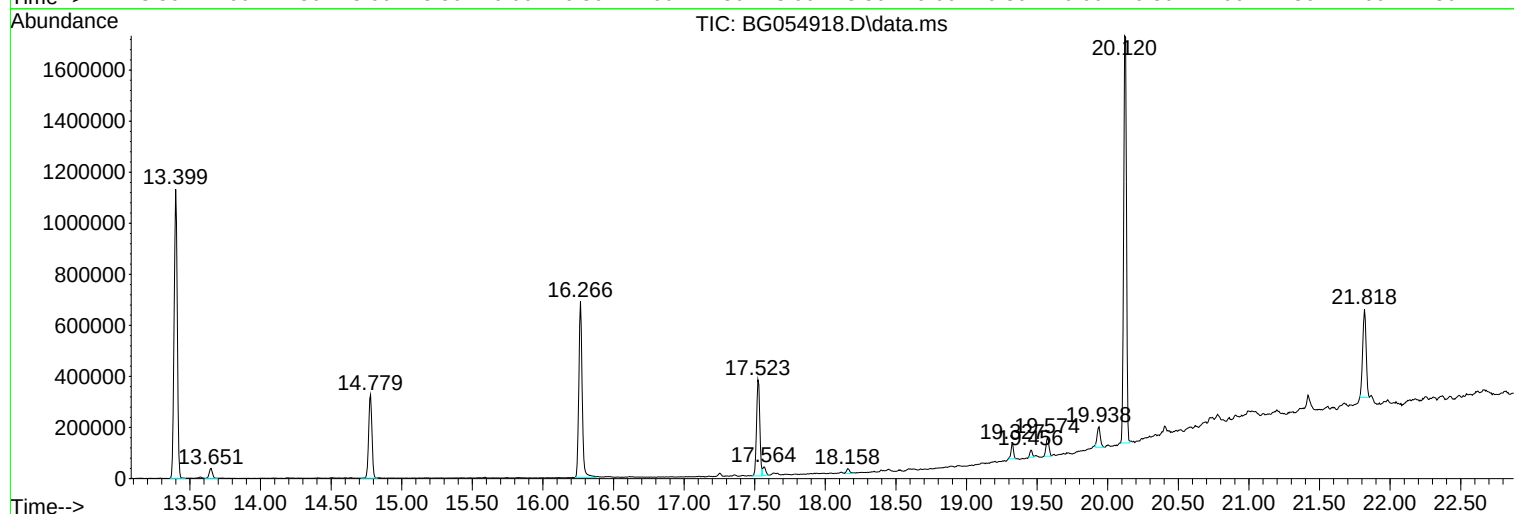
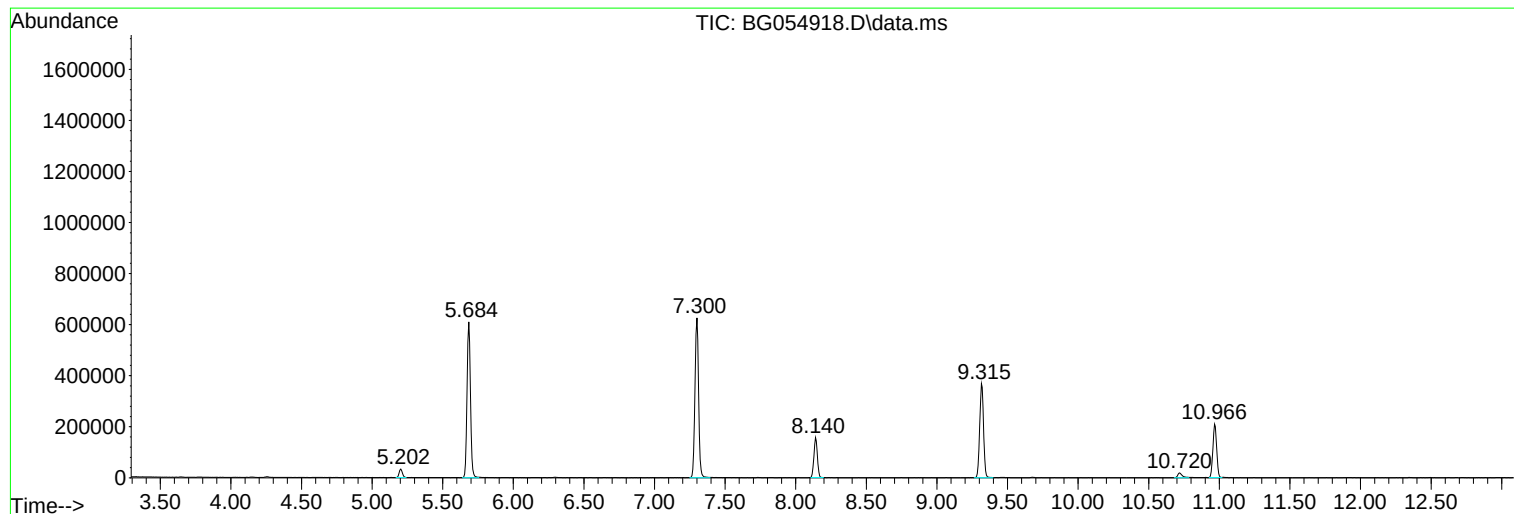
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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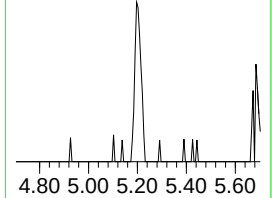
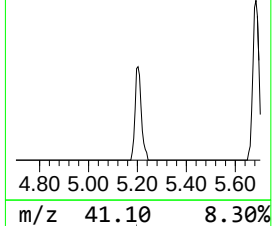
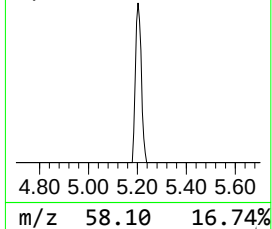
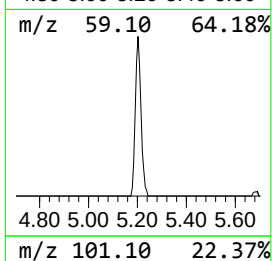
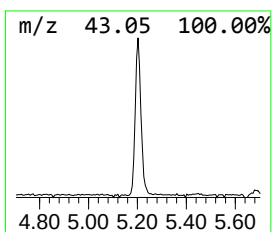
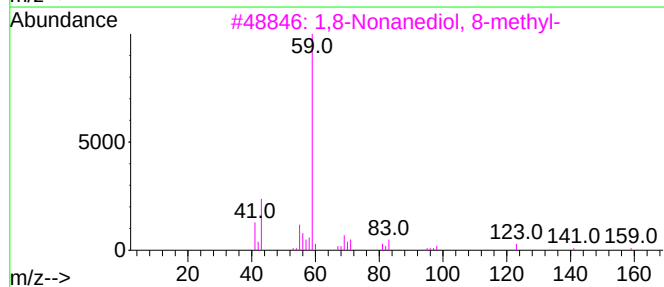
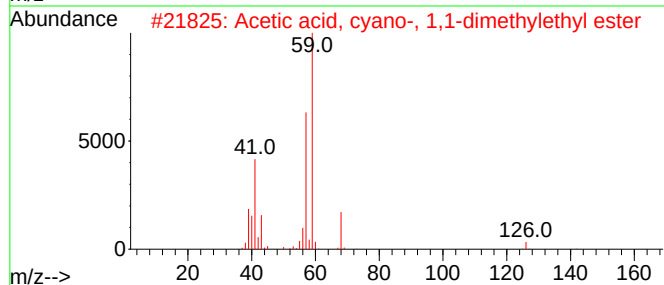
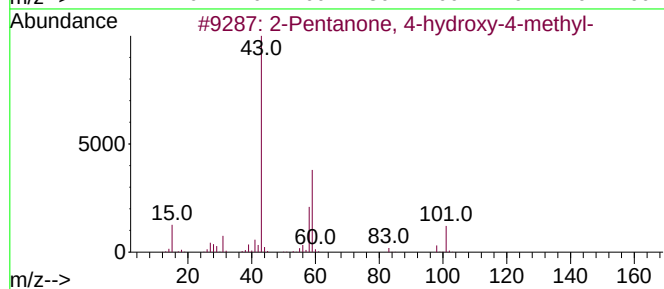
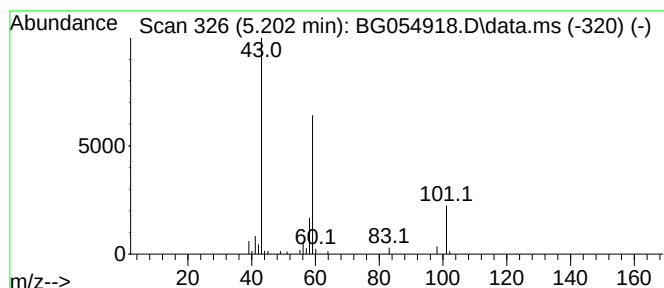
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.202	4.02 ng	53703	1,4-Dichlorobenzene-d4	8.140

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	39		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17		
3	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17		
4	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		



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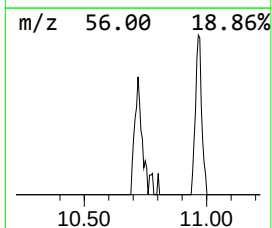
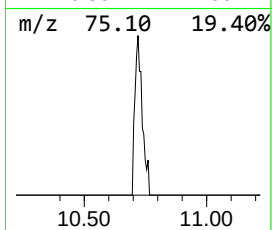
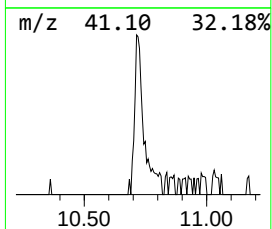
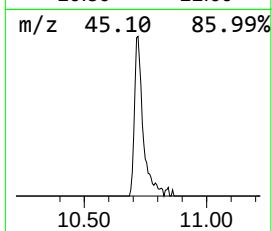
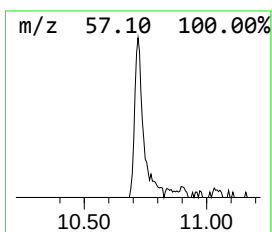
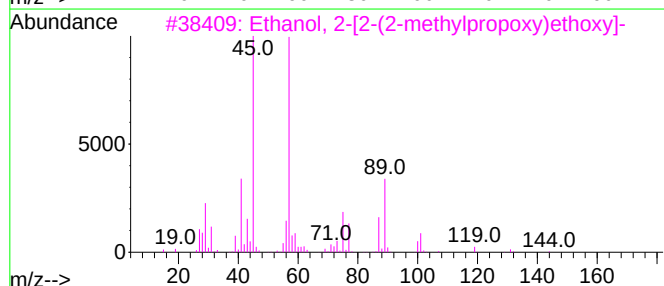
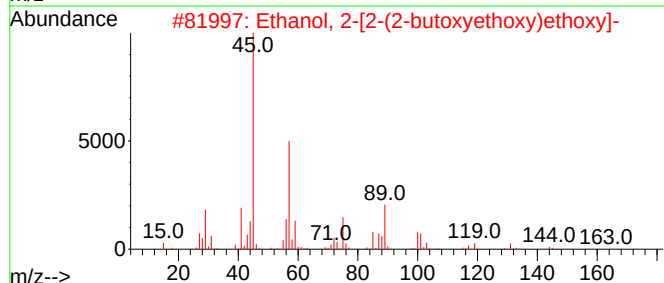
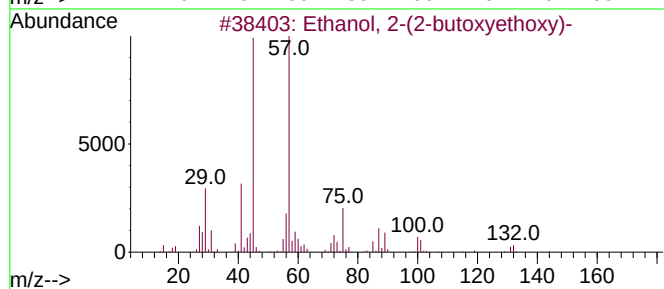
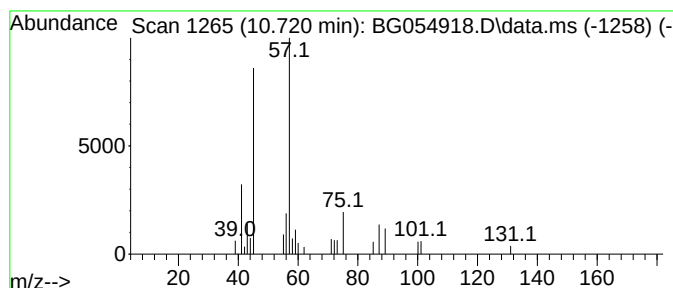
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.720	2.18 ng	41969	Naphthalene-d8	10.966

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-butoxyethoxy)et...	206	C10H22O4	000143-22-6	59
3		Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	50
4		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	45
5		Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	42



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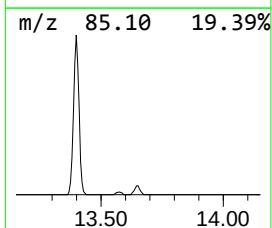
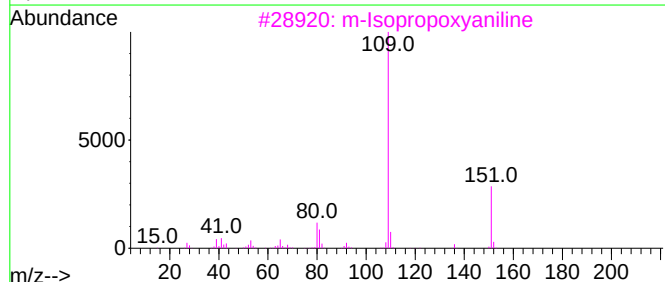
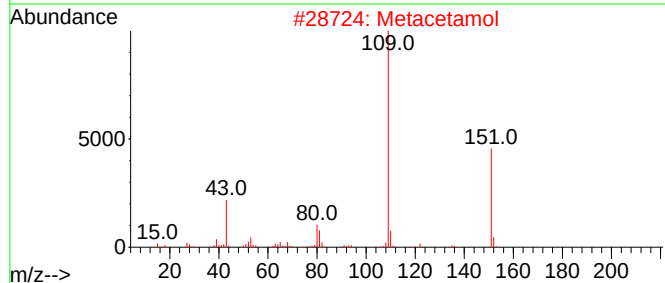
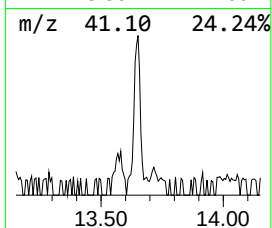
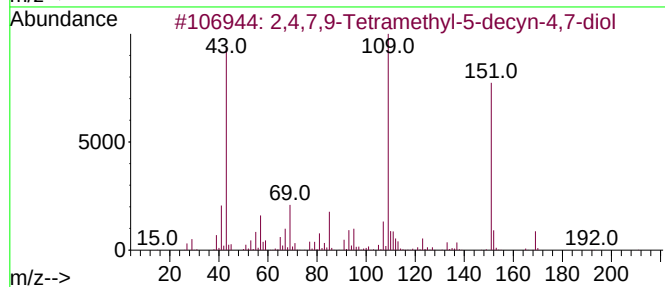
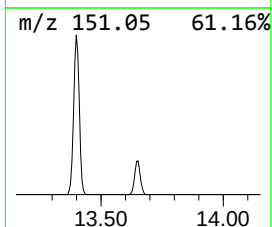
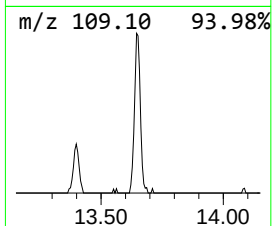
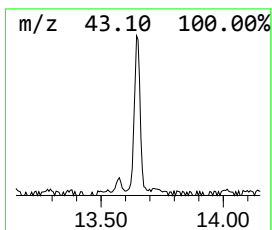
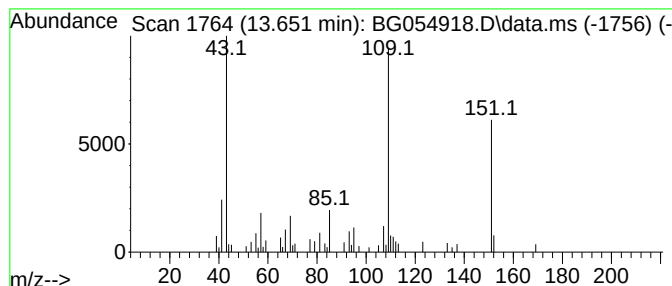
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
13.651	2.32 ng	62044	Acenaphthene-d10		14.780
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	91
2	Metacetamol	151	C8H9NO2	000621-42-1	52
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50
4	Acetaminophen	151	C8H9NO2	000103-90-2	50
5	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	50



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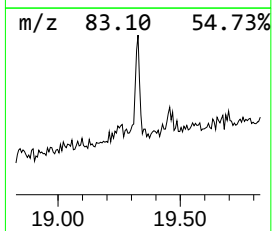
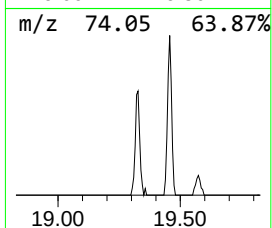
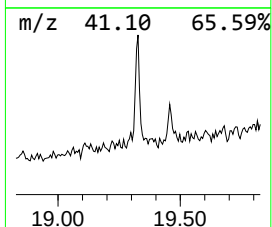
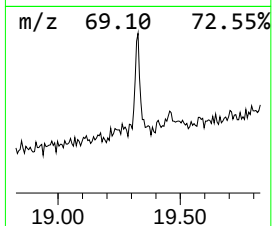
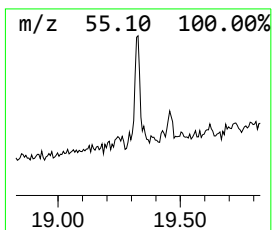
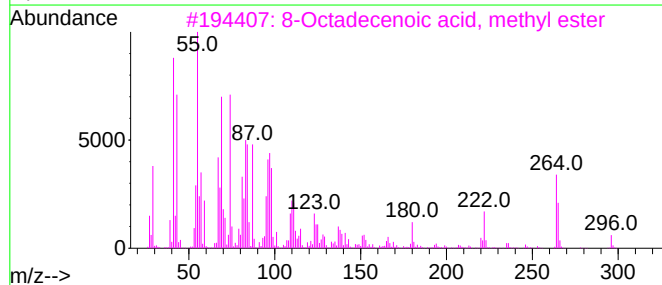
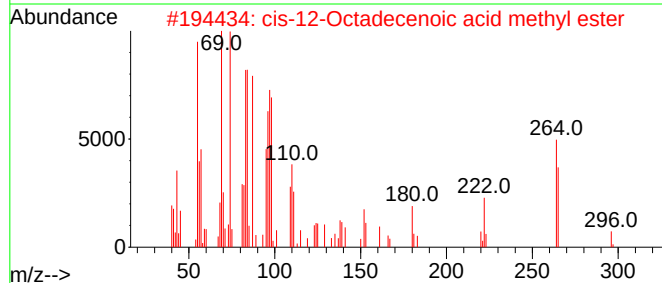
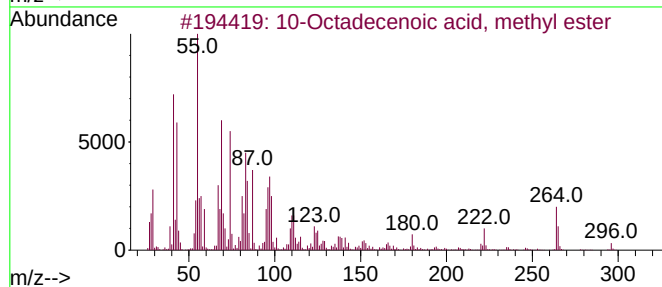
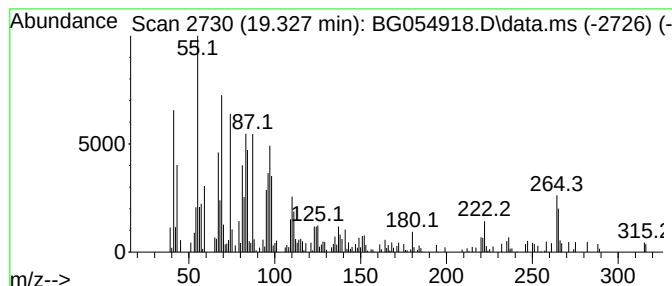
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Peak Number 4 10-Octadecenoic acid, methy... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.327	2.41 ng	72660	Phenanthrene-d10	17.523	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
2	cis-12-Octadecenoic acid methyl ...	296	C19H36O2	1000427-68-4	94
3	8-Octadecenoic acid, methyl ester	296	C19H36O2	002345-29-1	93
4	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	93
5	(Z)-15-Octadecenoic acid methyl ...	296	C19H36O2	1000427-69-3	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.202	4.0	ng	53703	1	8.140	267402	20.0
Ethanol, 2-(2-b...	10.720	2.2	ng	41969	2	10.966	385110	20.0
2,4,7,9-Tetrame...	13.651	2.3	ng	62044	3	14.780	534930	20.0
10-Octadecenoic...	19.327	2.4	ng	72660	4	17.523	604186	20.0