

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP080521\
 Data File : BP006526.D
 Acq On : 06 Aug 2021 02:36
 Operator : CG/JU
 Sample : M3268-12
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20210574-COM-47

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_P\Methods\8270E-BP080321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP006526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.911	305	310	321	rVB	656835	939087	12.35%	1.956%
2	5.358	380	386	400	rVB	3216240	4525495	59.50%	9.424%
3	5.969	486	490	496	rVB	136840	193245	2.54%	0.402%
4	6.934	647	654	664	rBV	3131563	4791166	62.99%	9.977%
5	7.758	787	794	802	rVB	920471	1482323	19.49%	3.087%
6	8.910	983	990	1000	rVB	1937830	3049517	40.09%	6.350%
7	10.328	1225	1231	1242	rBV	195400	329042	4.33%	0.685%
8	10.540	1259	1267	1274	rBV	1232393	2093496	27.52%	4.360%
9	13.010	1678	1687	1697	rBV	3811144	5531565	72.72%	11.519%
10	14.381	1912	1920	1928	rBV	1784586	2615586	34.39%	5.447%
11	15.875	2164	2174	2190	rBV	3247911	4692434	61.69%	9.772%
12	17.133	2381	2388	2400	rBV	2172275	3055581	40.17%	6.363%
13	18.039	2538	2542	2549	rBV	106409	154790	2.04%	0.322%
14	19.710	2820	2826	2833	rBV	6541251	7606305	100.00%	15.840%
15	20.957	3034	3038	3045	rBV	258652	349082	4.59%	0.727%
16	21.233	3080	3085	3090	rBV	2477117	3225742	42.41%	6.717%
17	23.557	3473	3480	3491	rVB2	1741762	3386334	44.52%	7.052%

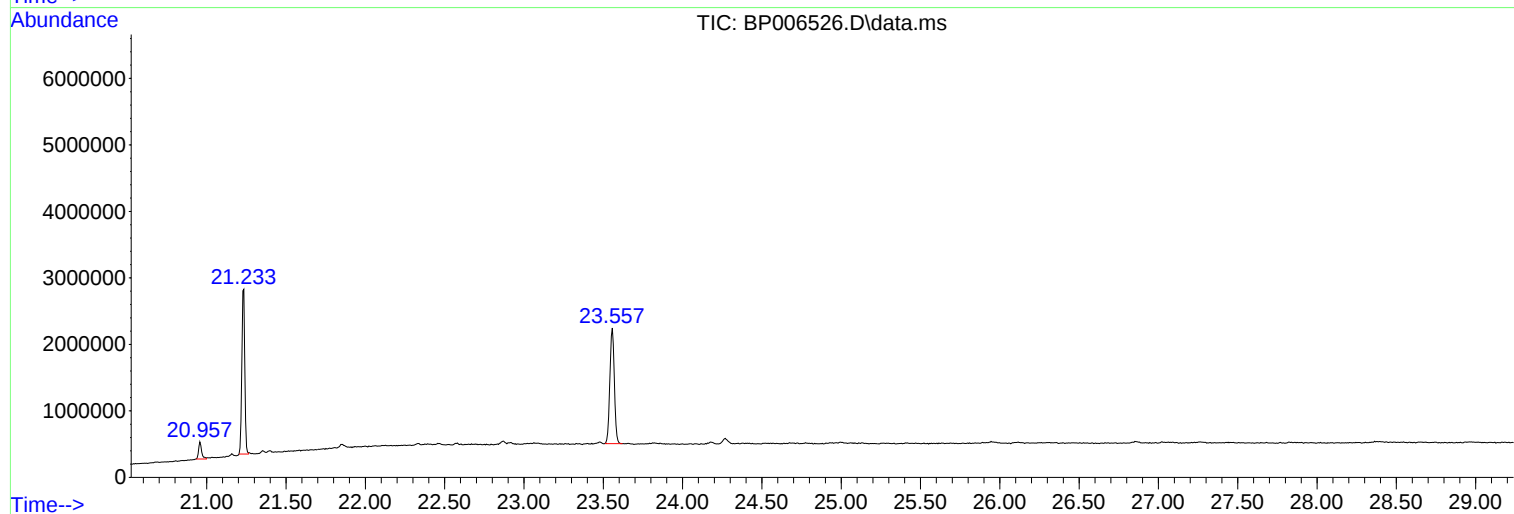
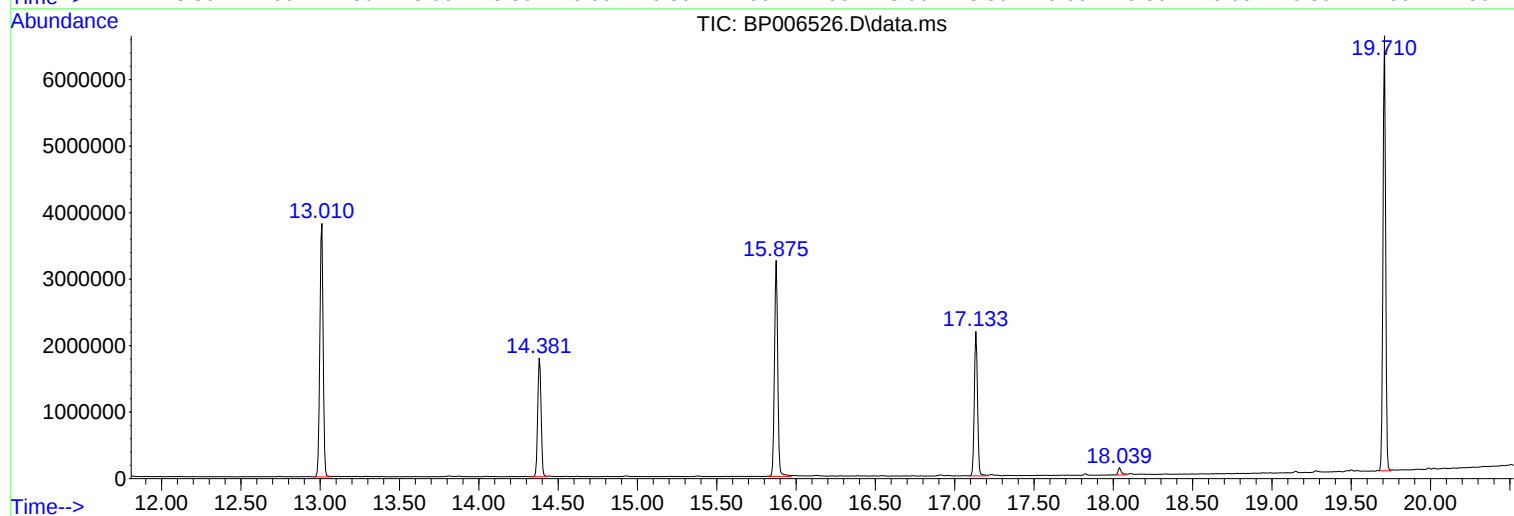
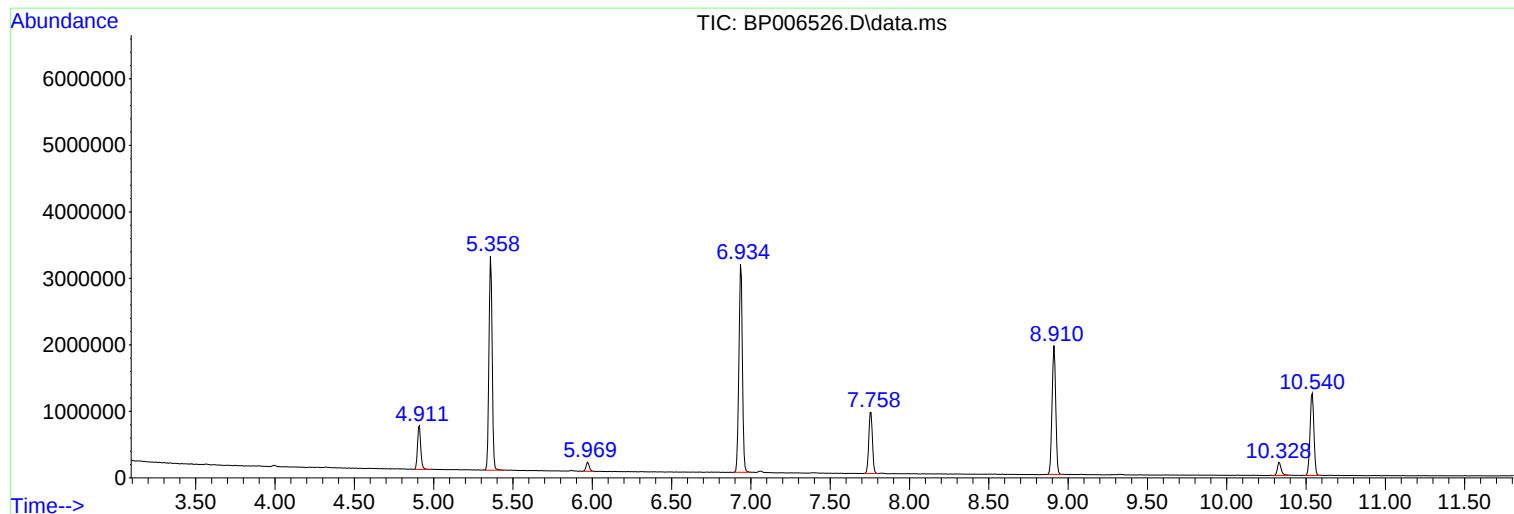
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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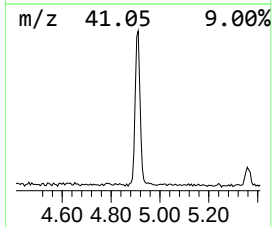
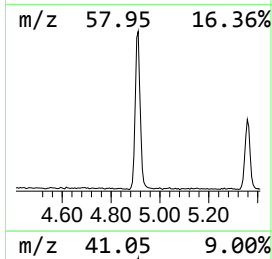
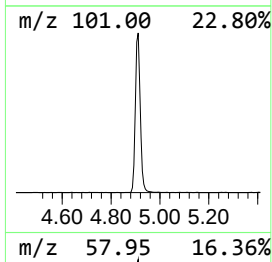
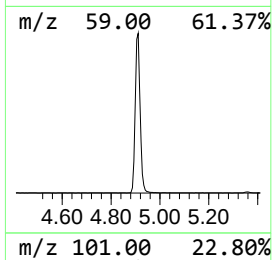
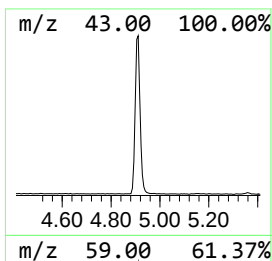
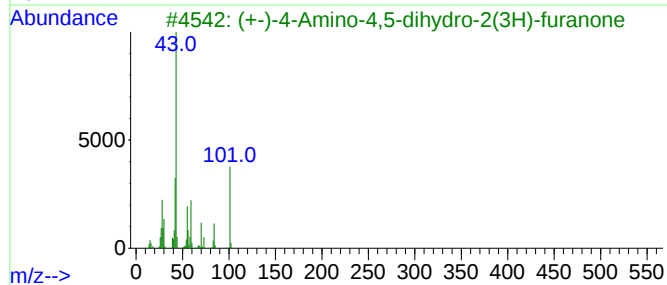
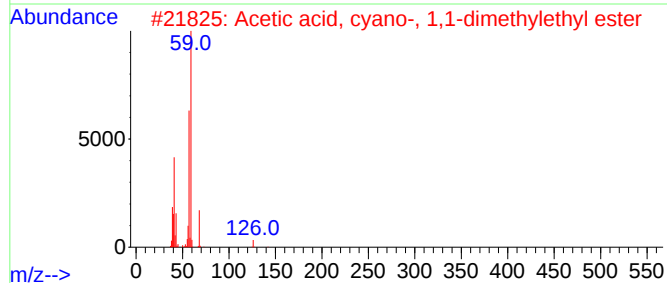
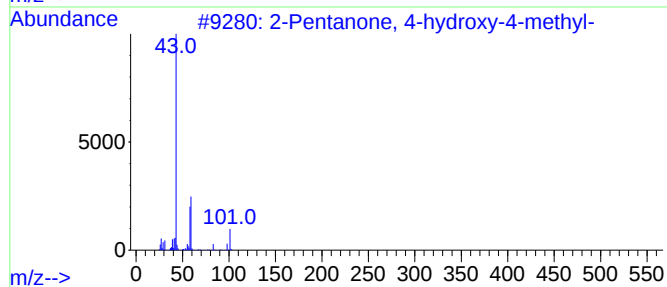
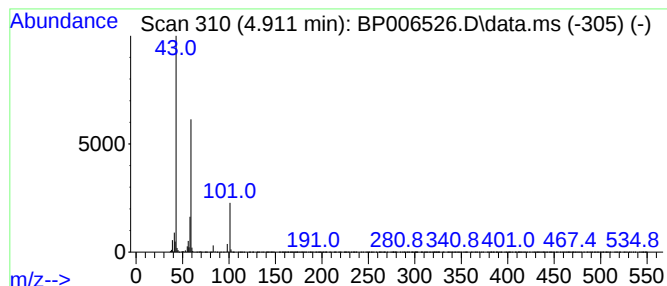
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP080321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.911	12.67 ng	939087	1,4-Dichlorobenzene-d4	7.758

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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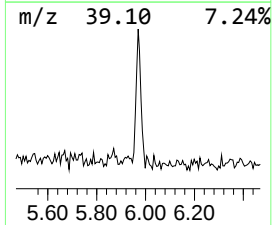
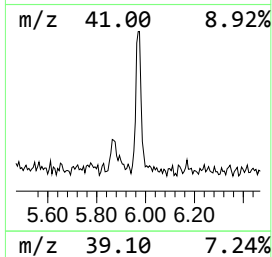
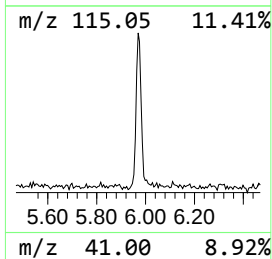
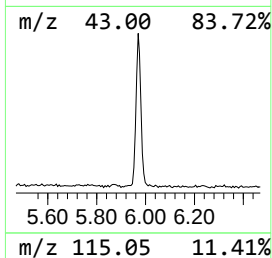
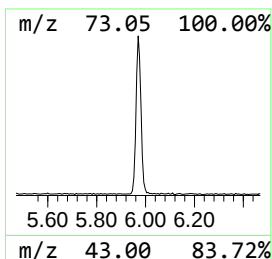
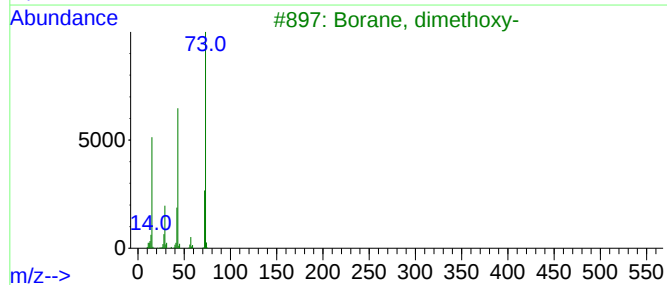
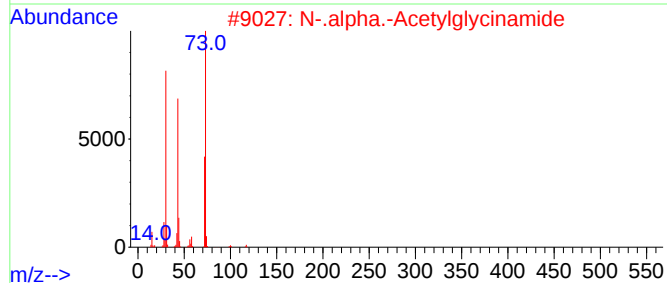
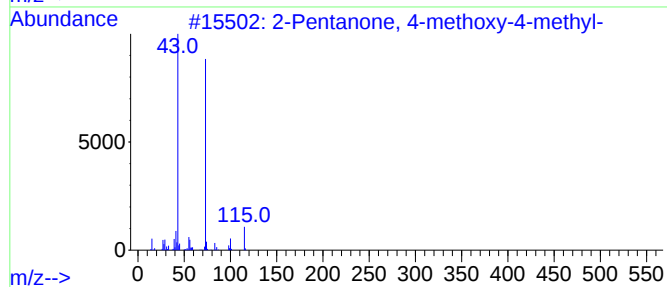
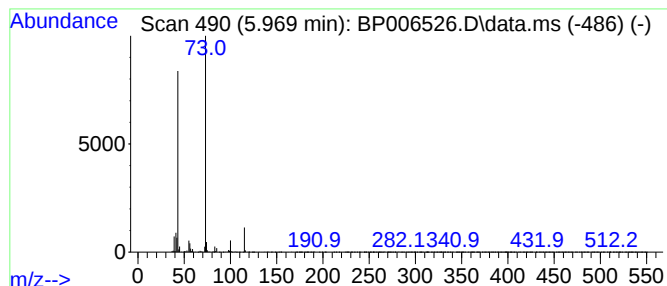
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Peak Number 2 2-Pentanone, 4-methoxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.969	2.61 ng	193245	1,4-Dichlorobenzene-d4	7.758

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			N-.alpha.-Acetylglycinamide	116	C4H8N2O2	002620-63-5	50
3			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	40
4			4-Acetoxytridecane	242	C15H30O2	060826-30-4	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	16



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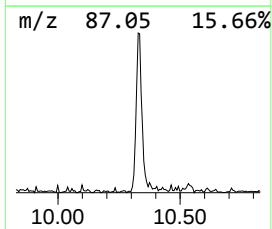
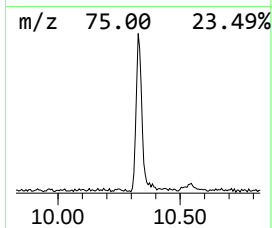
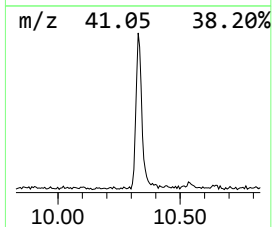
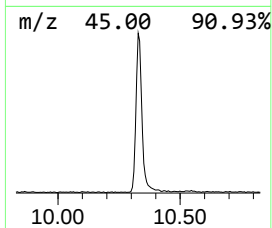
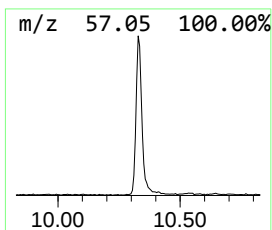
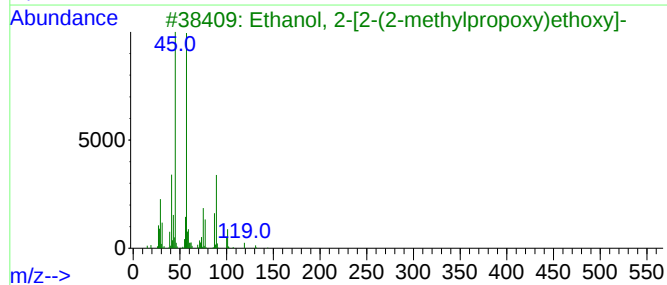
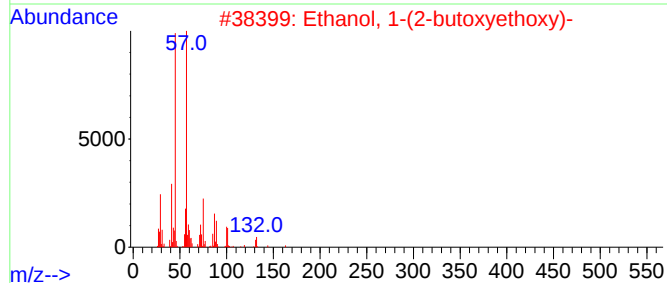
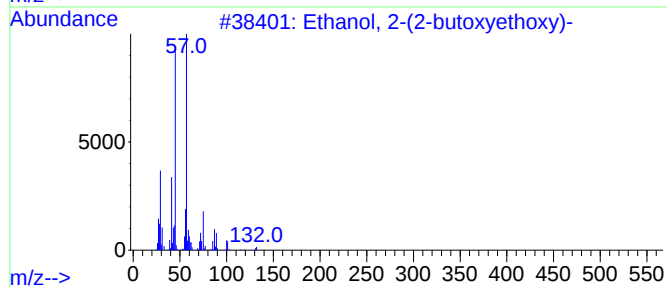
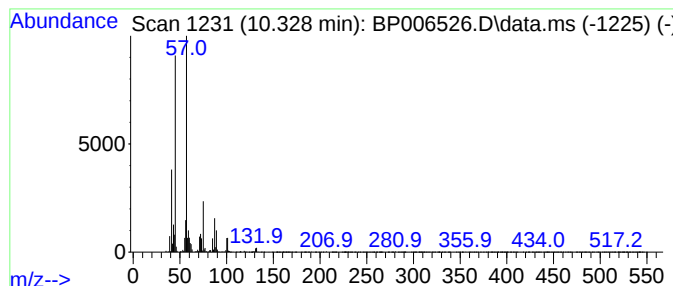
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Peak Number 3 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.328	3.14 ng	329042	Naphthalene-d8	10.540

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	52



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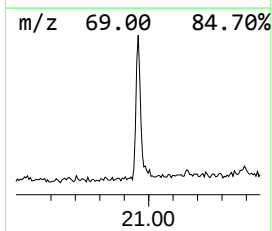
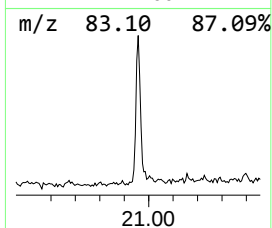
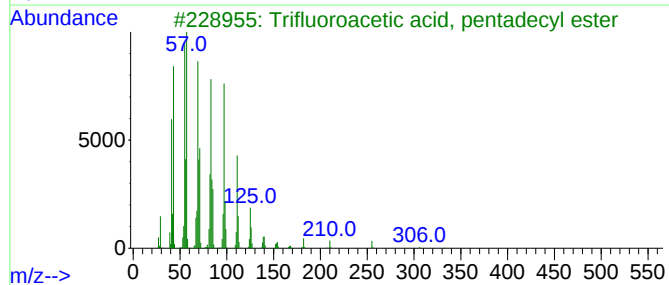
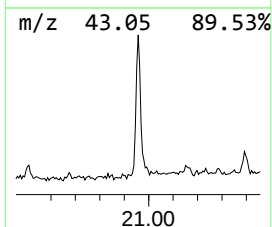
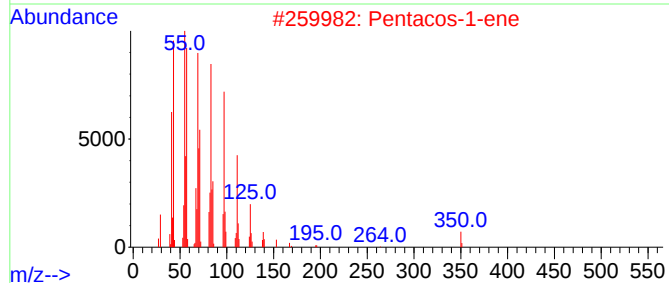
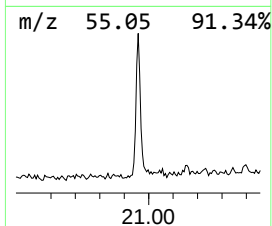
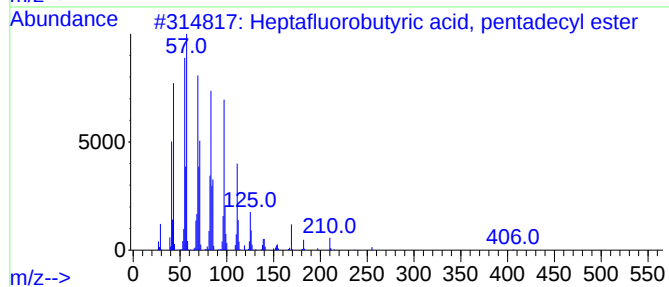
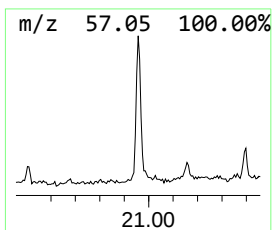
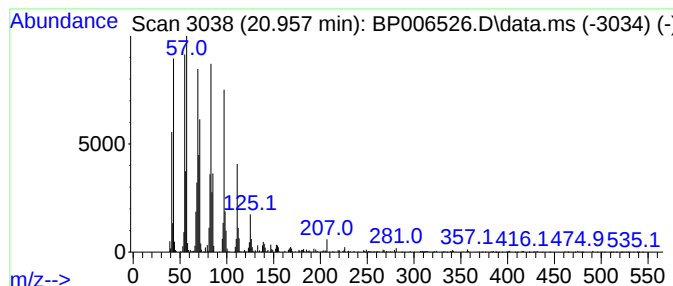
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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	2.16 ng	349082	Chrysene-d12	21.233

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			Pentacos-1-ene	350	C25H50	016980-85-1	94
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
4			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
5			Octacosanol	410	C28H58O	000557-61-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.911	12.7	ng	939087	1	7.758	1482320	20.0
2-Pentanone, 4-...	5.969	2.6	ng	193245	1	7.758	1482320	20.0
Ethanol, 2-(2-b...	10.328	3.1	ng	329042	2	10.540	2093500	20.0
Heptafluorobuty...	20.957	2.2	ng	349082	5	21.233	3225740	20.0