

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101823\
 Data File : BF135878.D
 Acq On : 19 Oct 2023 07:00
 Operator : CG\JU
 Sample : 04765-03 2X
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TT-2

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-BF101323.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.334	378	382	395	rBV	9840	23413	3.18%	0.350%
2	4.951	483	487	499	rBV	536445	596372	80.94%	8.914%
3	5.381	557	560	586	rBV	502806	680707	92.39%	10.174%
4	5.757	621	624	631	rVB	13275	15126	2.05%	0.226%
5	6.398	730	733	759	rBV	502851	648585	88.03%	9.694%
6	6.739	788	791	803	rBV	386633	331839	45.04%	4.960%
7	7.304	884	887	901	rBV	397779	382504	51.91%	5.717%
8	8.016	1005	1008	1021	rVB	468960	425476	57.75%	6.359%
9	9.092	1188	1191	1200	rVB	833482	736793	100.00%	11.012%
10	9.169	1200	1204	1208	rVV3	9253	13037	1.77%	0.195%
11	9.216	1208	1212	1223	rVB	247200	247095	33.54%	3.693%
12	9.375	1235	1239	1243	rBV6	7395	10893	1.48%	0.163%
13	9.639	1280	1284	1287	rBV2	6733	9060	1.23%	0.135%
14	9.775	1304	1307	1312	rBV	456819	384754	52.22%	5.751%
15	10.574	1440	1443	1453	rBV	368183	334301	45.37%	4.997%
16	10.869	1488	1493	1498	rBV6	4621	10333	1.40%	0.154%
17	11.157	1540	1542	1548	rVB5	6085	8282	1.12%	0.124%
18	11.274	1558	1562	1565	rBV	369663	316233	42.92%	4.727%
19	11.804	1650	1652	1660	rBV3	45341	62536	8.49%	0.935%
20	12.339	1737	1743	1744	rBV5	7701	11554	1.57%	0.173%
21	12.374	1744	1749	1752	rVV5	20060	23463	3.18%	0.351%
22	12.504	1768	1771	1772	rBV	26921	28258	3.84%	0.422%
23	12.527	1772	1775	1784	rVV7	27370	60080	8.15%	0.898%
24	12.598	1784	1787	1793	rVV7	19402	27123	3.68%	0.405%
25	12.733	1805	1810	1816	rVB	31648	40137	5.45%	0.600%
26	12.868	1829	1833	1841	rVB	773479	639960	86.86%	9.565%
27	13.439	1927	1930	1933	rBV4	11912	18398	2.50%	0.275%
28	13.939	2012	2015	2019	rBV	346017	338367	45.92%	5.057%
29	15.421	2263	2267	2275	rBV	180466	247024	33.53%	3.692%
30	16.939	2524	2525	2526	rBV	28042	18929	2.57%	0.283%

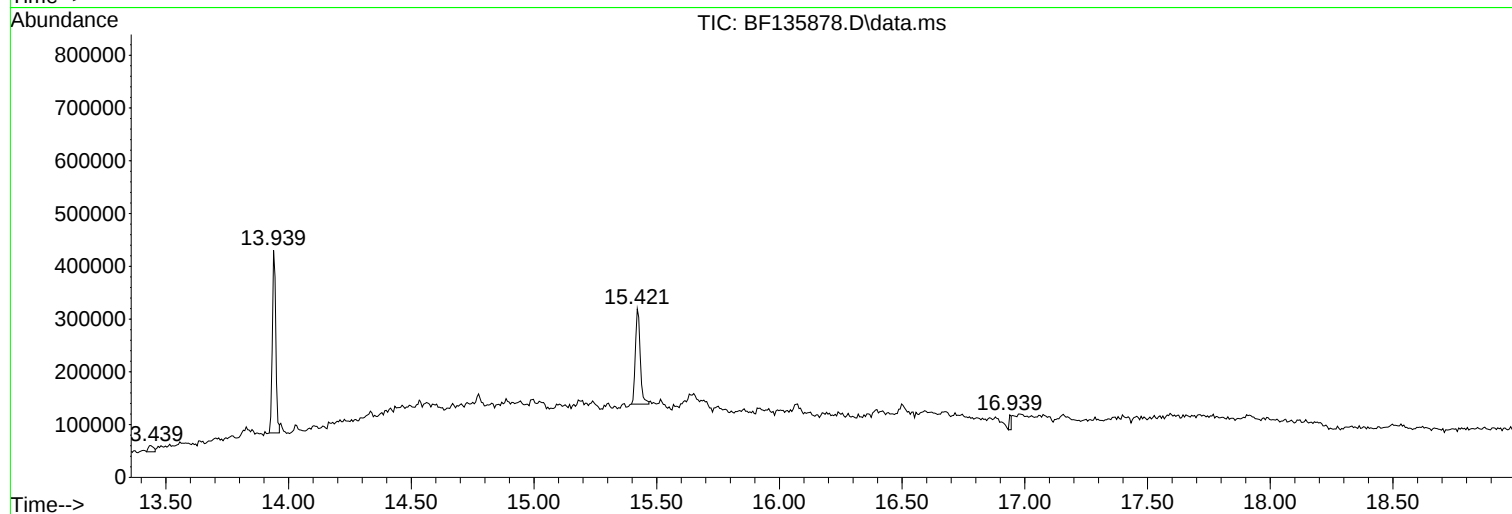
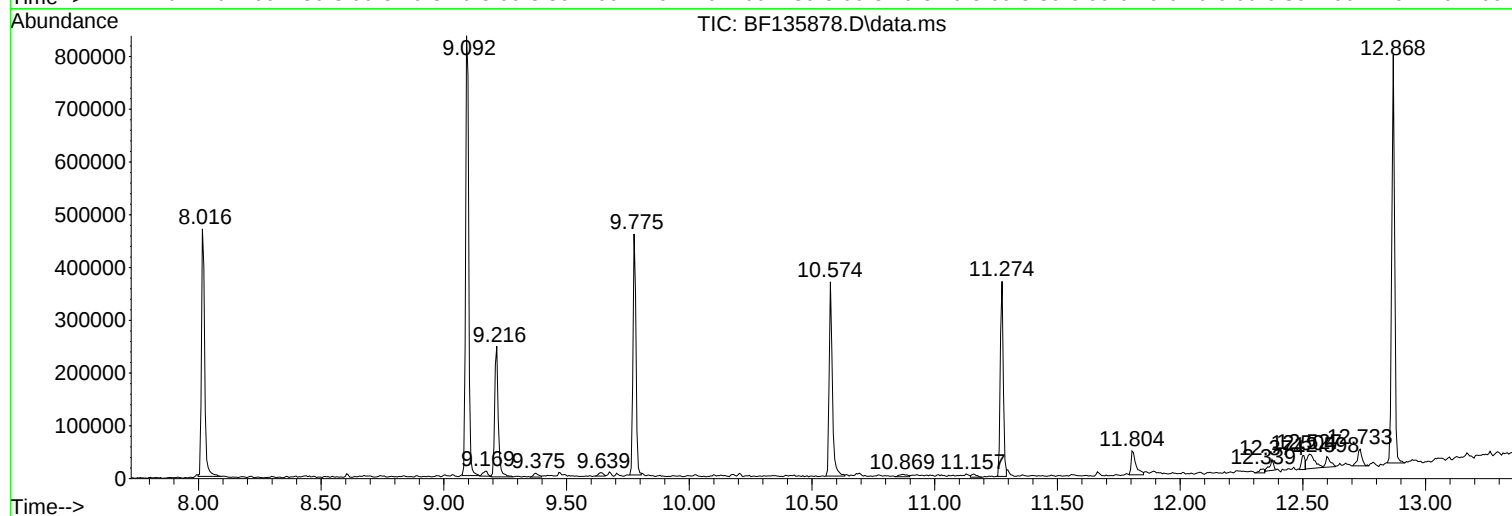
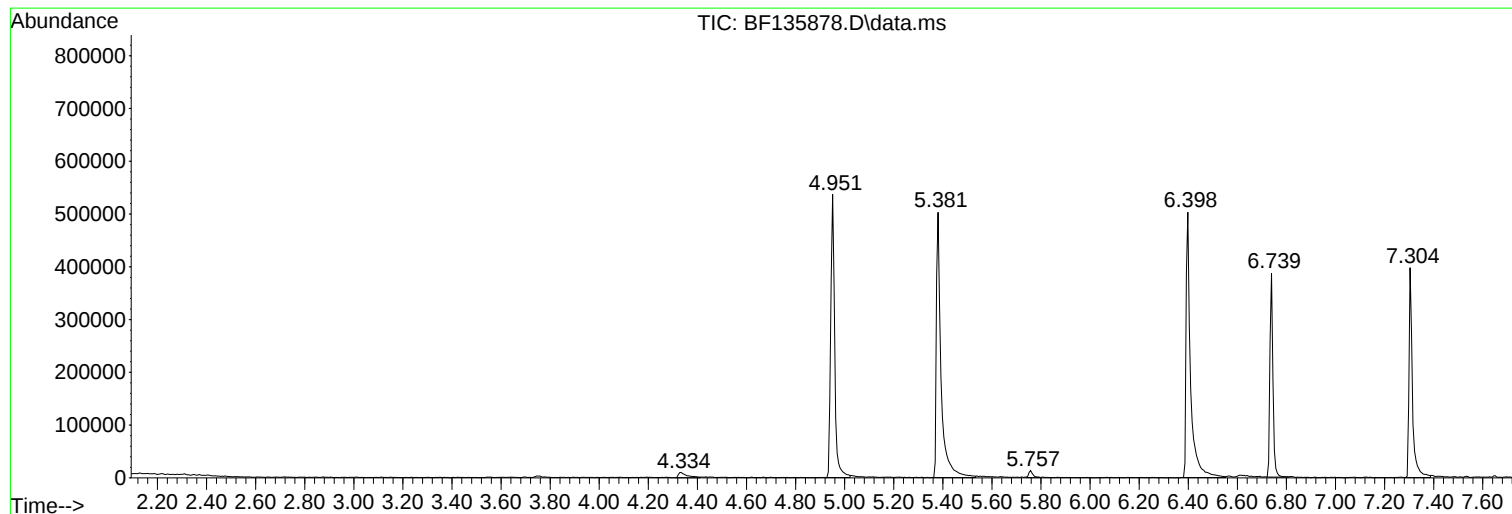
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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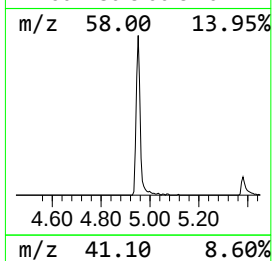
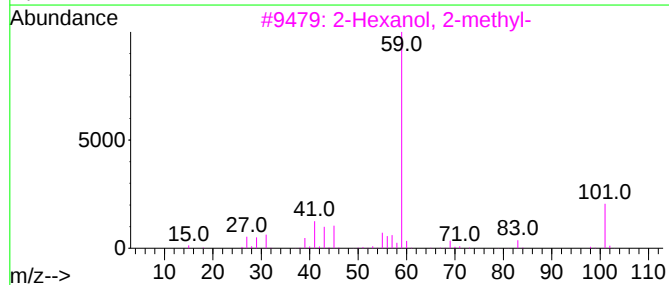
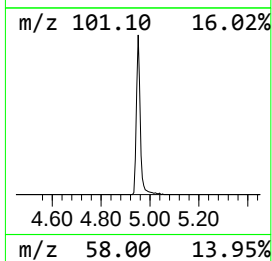
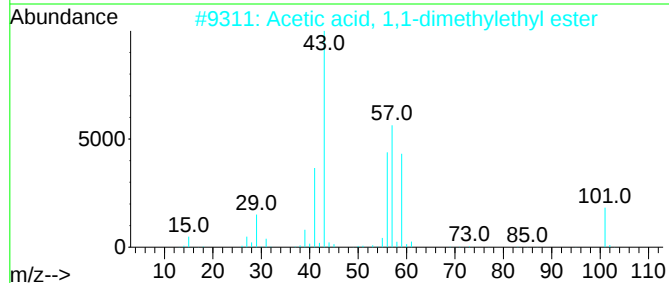
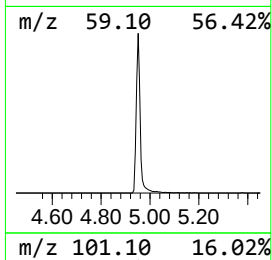
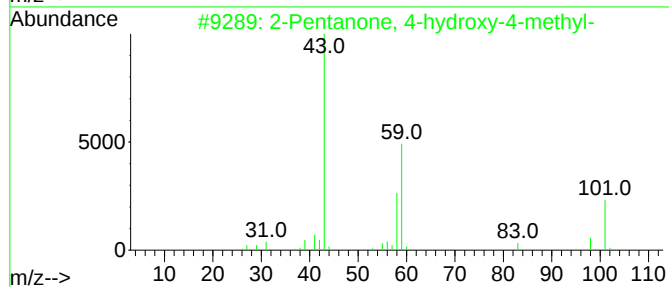
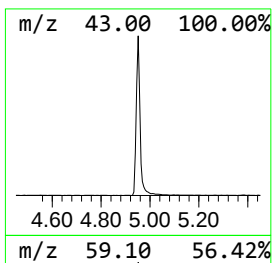
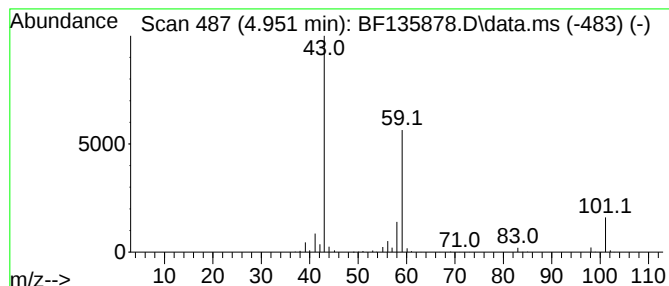
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.951	35.94 ng	596372	1,4-Dichlorobenzene-d4	6.739

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
4	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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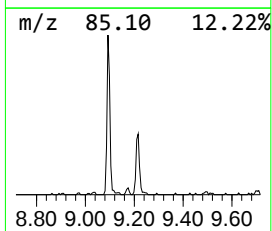
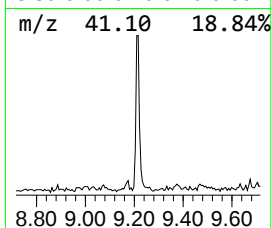
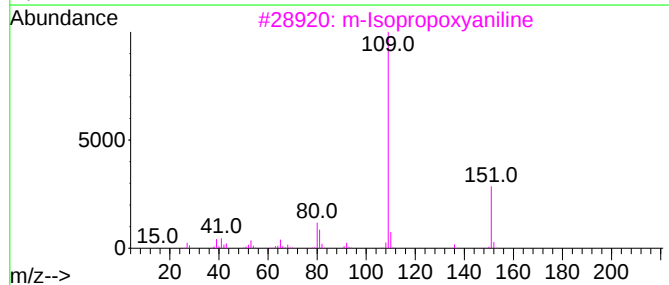
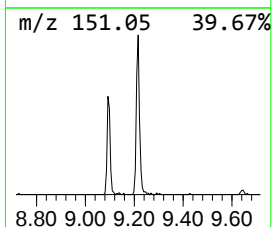
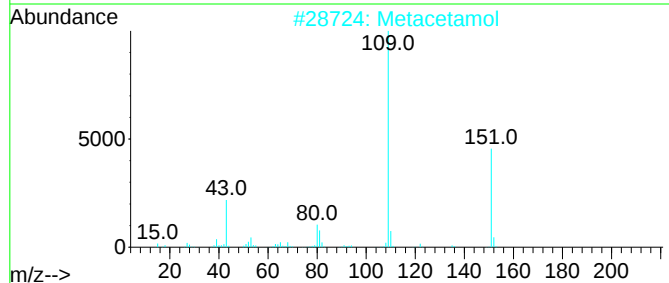
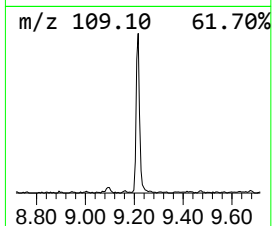
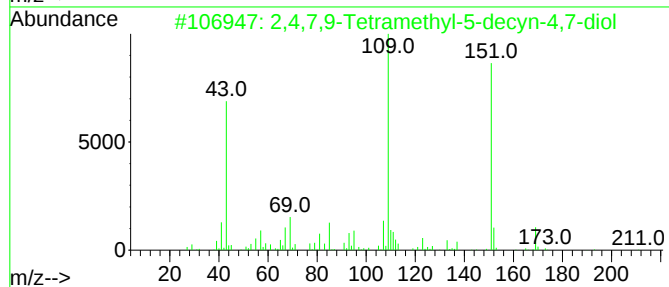
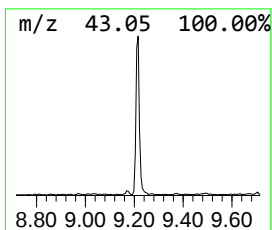
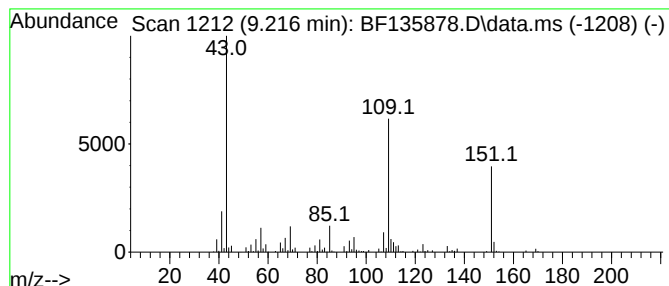
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.216	12.84 ng	247095	Acenaphthene-d10	9.775

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90	
2	Metacetamol	151	C8H9NO2	000621-42-1	52	
3	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	50	
4	N-Cyclopropyl-p-fluorobenzylamine	165	C10H12FN	1000250-88-9	35	
5	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	35	



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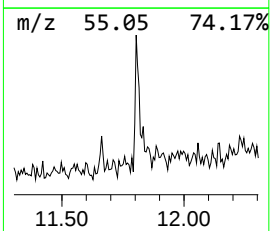
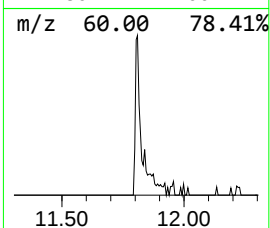
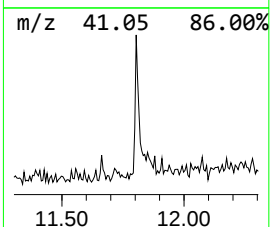
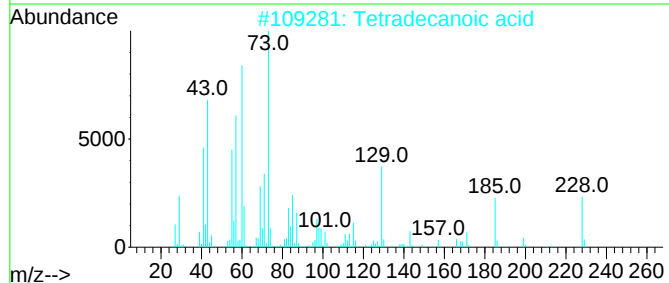
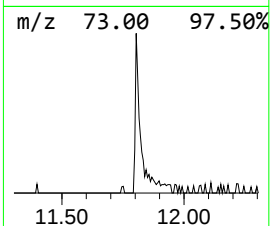
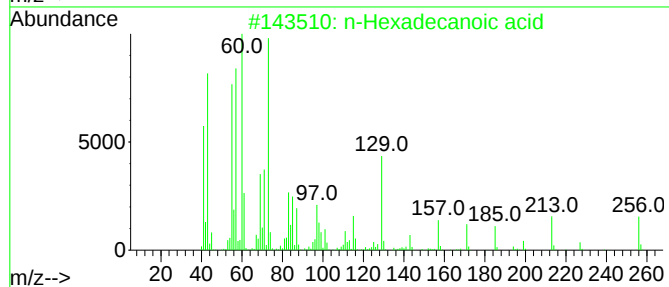
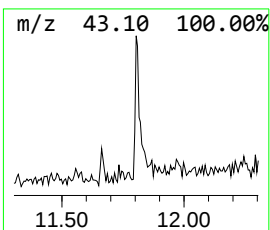
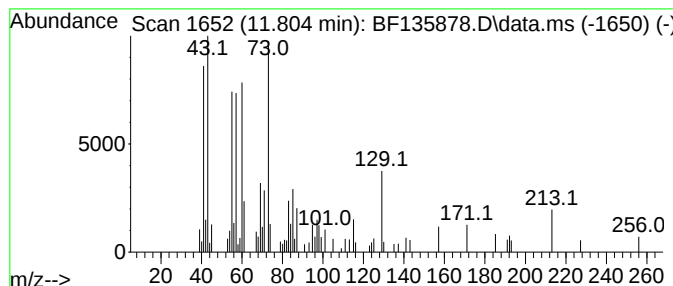
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	3.96 ng	62536	Phenanthrene-d10	11.274

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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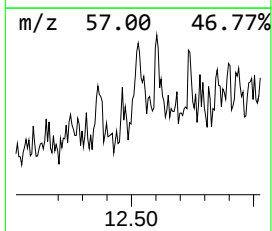
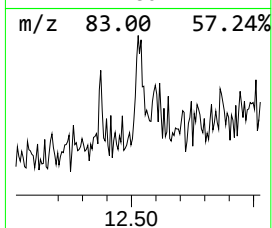
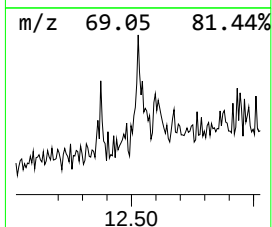
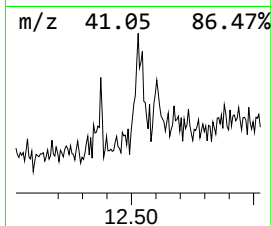
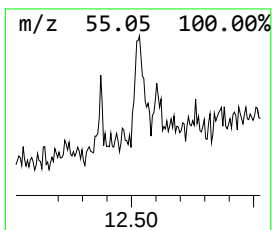
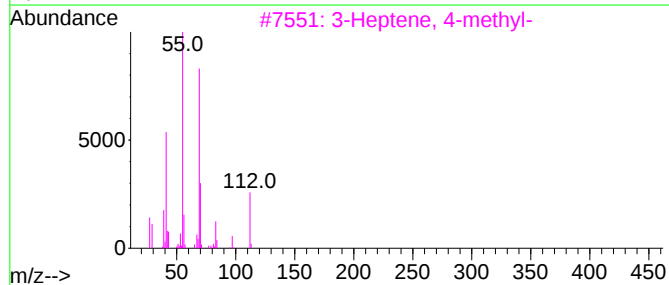
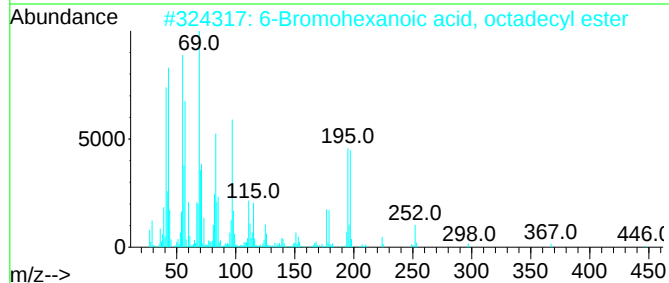
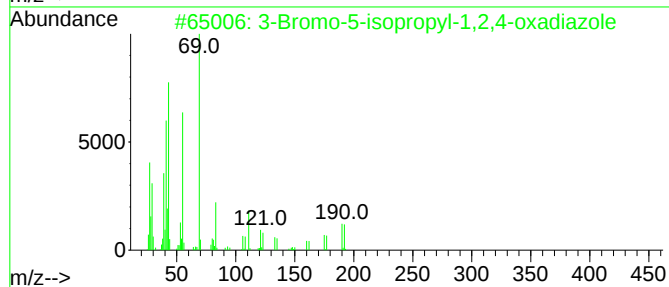
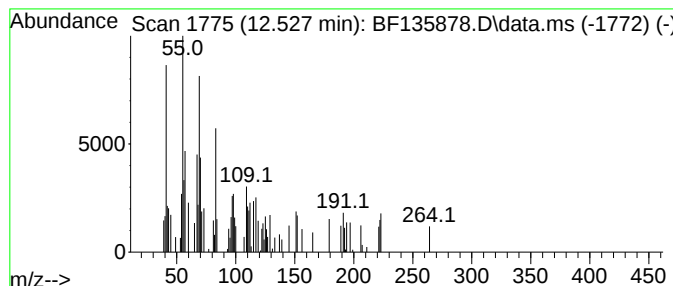
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown12.527 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.527	3.80 ng	60080	Phenanthrene-d10	11.274

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Bromo-5-isopropyl-1,2,4-oxadia...	190	C5H7BrN2O	121562-07-0	43
2			6-Bromohexanoic acid, octadecyl ...	446	C24H47BrO2	1000281-92-1	43
3			3-Heptene, 4-methyl-	112	C8H16	004485-16-9	43
4			Acetic acid, trifluoro-, undecyl...	268	C13H23F3O2	053800-01-4	38
5			2-Buten-1-one, 1-(2,6,6-trimethy...	192	C13H20O	024720-09-0	38



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.951	35.9	ng	596372	1	6.739	331839	20.0
2,4,7,9-Tetrame...	9.216	12.8	ng	247095	3	9.775	384754	20.0
n-Hexadecanoic ...	11.804	4.0	ng	62536	4	11.274	316233	20.0
unknown12.527	12.527	3.8	ng	60080	4	11.274	316233	20.0