

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101623\
 Data File : BF135784.D
 Acq On : 16 Oct 2023 19:18
 Operator : CG\JU
 Sample : 04656-22
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 MW-1021

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: BF135784.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.299	29	36	52	rBV	153922	262342	8.16%	1.432%
2	4.428	394	398	409	rBV	163952	225272	7.01%	1.230%
3	4.957	485	488	496	rBV	54481	80491	2.50%	0.439%
4	5.369	555	558	583	rBV	1014948	1315850	40.92%	7.183%
5	6.387	728	731	749	rBV	510762	788745	24.53%	4.306%
6	6.581	762	764	775	rBV	77345	125361	3.90%	0.684%
7	6.734	787	790	804	rVB	645842	568152	17.67%	3.102%
8	7.304	884	887	906	rBV	1996123	1985749	61.76%	10.840%
9	8.016	1005	1008	1017	rBV	876444	734921	22.86%	4.012%
10	9.098	1188	1192	1195	rBV	3610300	3215385	100.00%	17.553%
11	9.216	1208	1212	1229	rVB	1142963	1111723	34.58%	6.069%
12	9.775	1303	1307	1317	rVB	960128	795491	24.74%	4.343%
13	10.575	1439	1443	1458	rBV	1993017	1968422	61.22%	10.746%
14	10.698	1462	1464	1474	rVB	40602	52008	1.62%	0.284%
15	11.269	1558	1561	1571	rBV	986789	854709	26.58%	4.666%
16	11.804	1649	1652	1664	rBV2	98392	147546	4.59%	0.805%
17	12.522	1767	1774	1777	rBV	86092	76380	2.38%	0.417%
18	12.598	1784	1787	1798	rBV4	21872	43901	1.37%	0.240%
19	12.869	1828	1833	1836	rBV	3115941	2869788	89.25%	15.666%
20	13.863	1996	2002	2004	rBV6	17453	34473	1.07%	0.188%
21	13.939	2011	2015	2025	rVB	490955	522256	16.24%	2.851%
22	15.410	2261	2265	2276	rBV	363098	539054	16.76%	2.943%

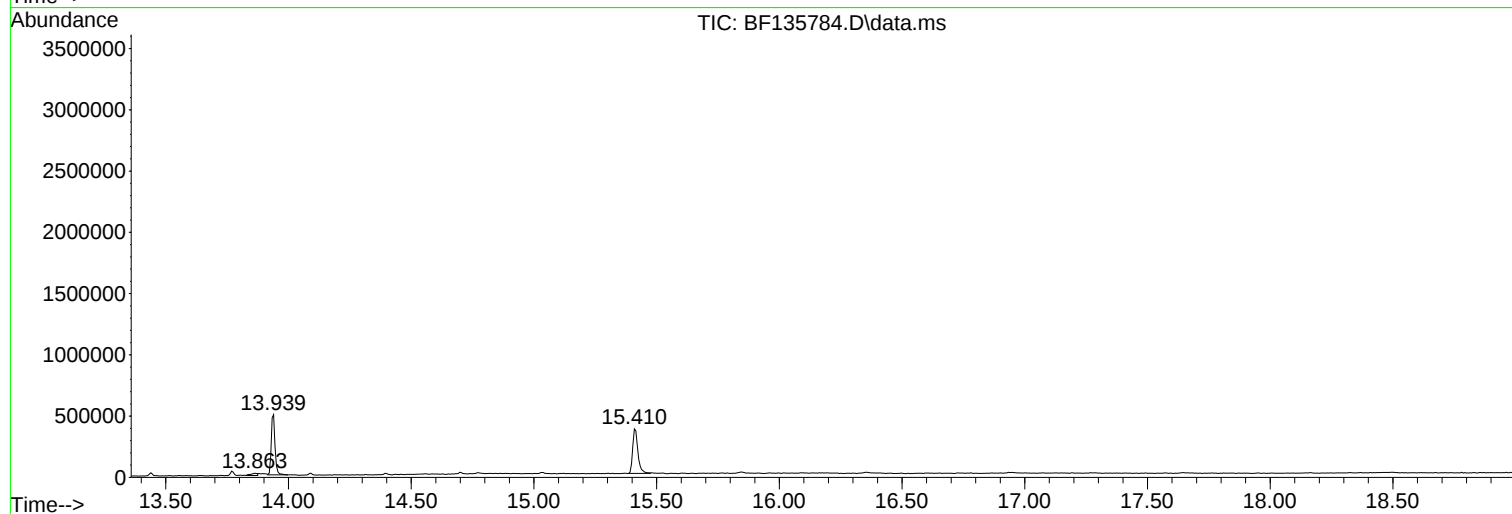
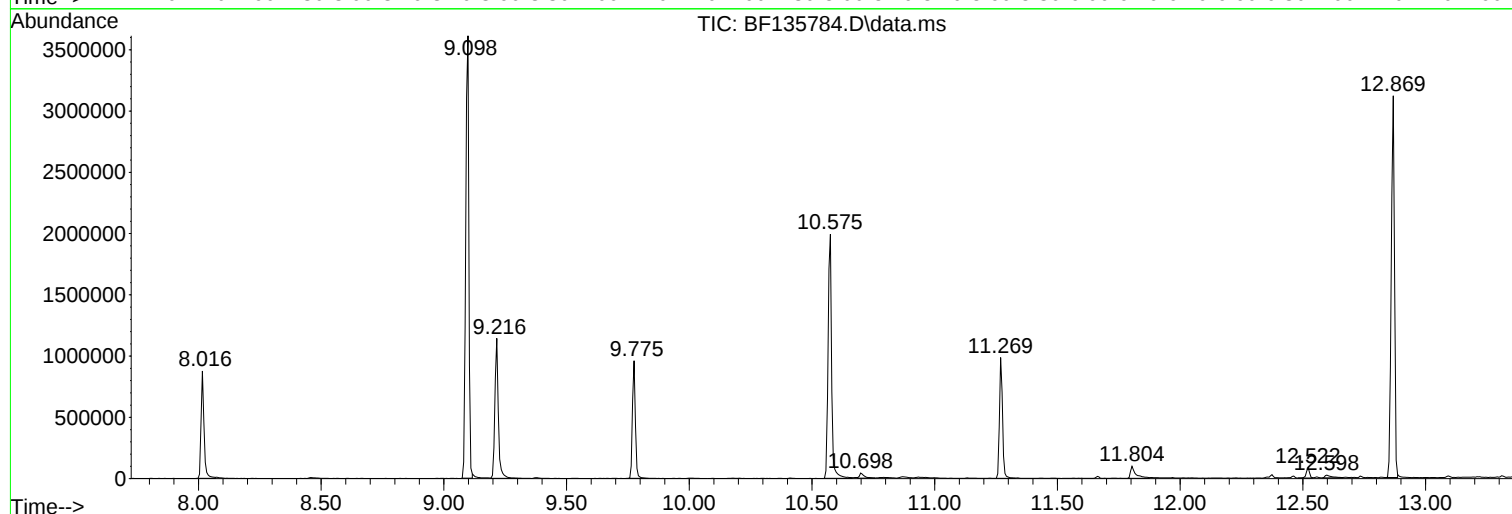
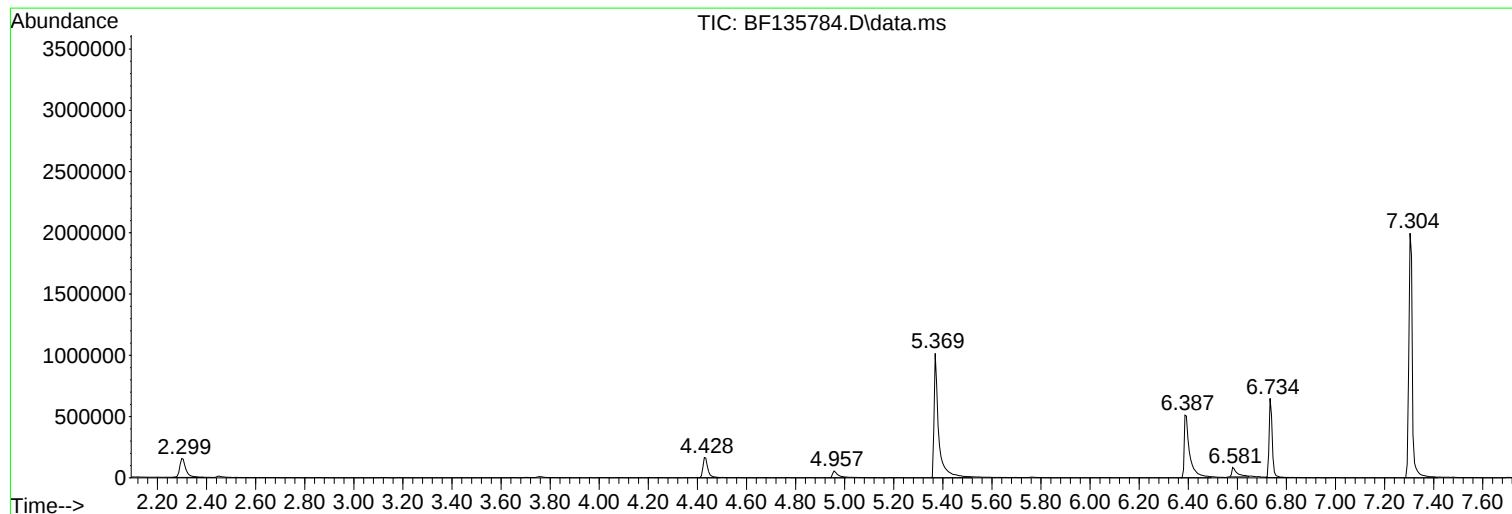
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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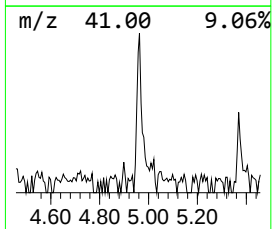
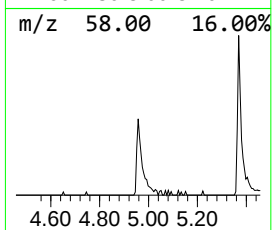
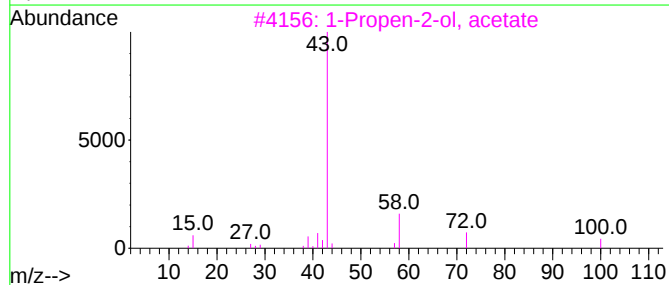
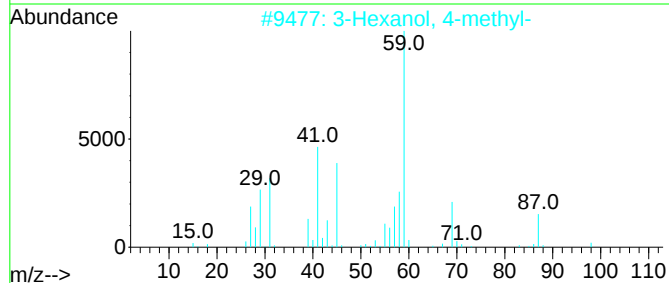
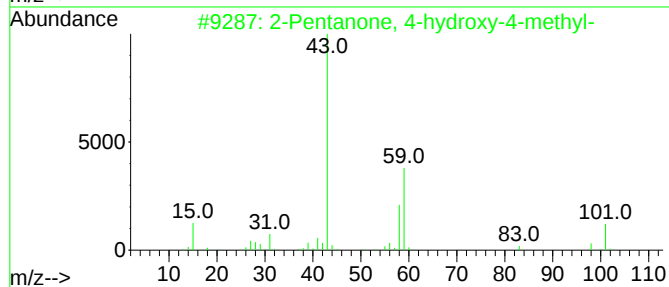
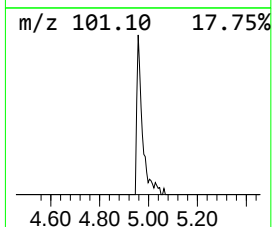
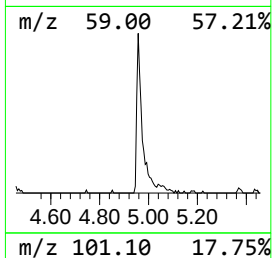
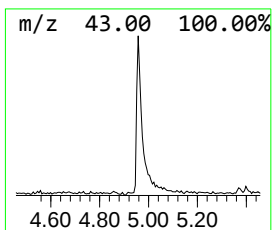
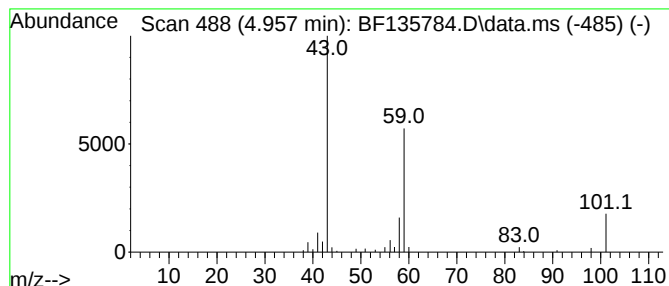
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101323.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.957	2.83 ng	80491	1,4-Dichlorobenzene-d4	6.734

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9	
5	5-Oxohexanenitrile	111	C6H9NO	010412-98-3	9	



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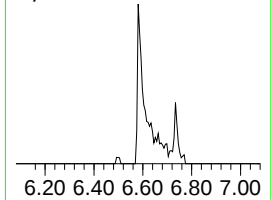
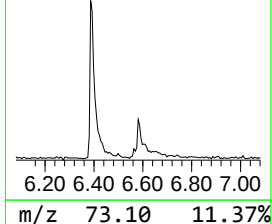
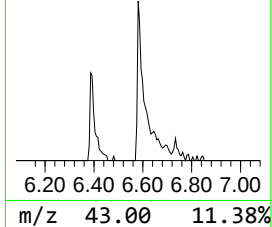
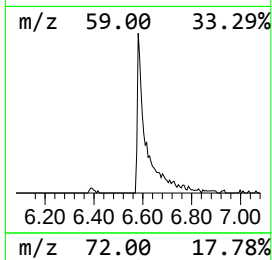
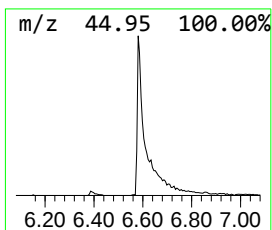
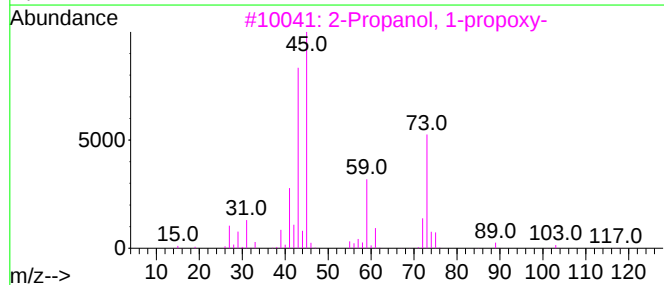
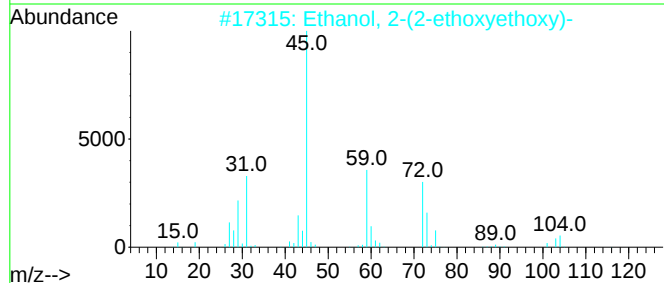
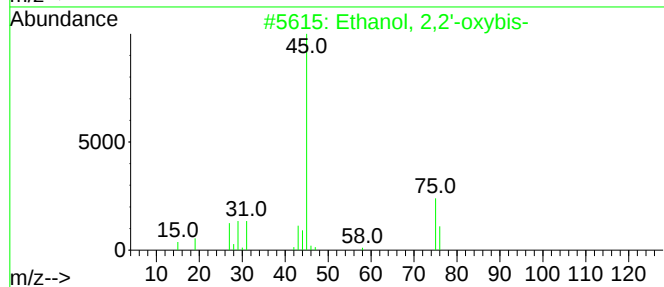
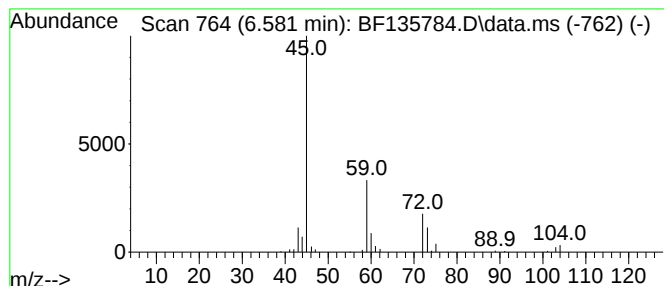
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Peak Number 4 Ethanol, 2,2'-oxybis- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.581	4.41 ng	125361	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2,2'-oxybis-	106	C4H10O3	000111-46-6	50
2			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	50
3			2-Propanol, 1-propoxy-	118	C6H14O2	001569-01-3	39
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	39
5			Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	39



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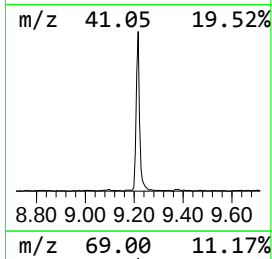
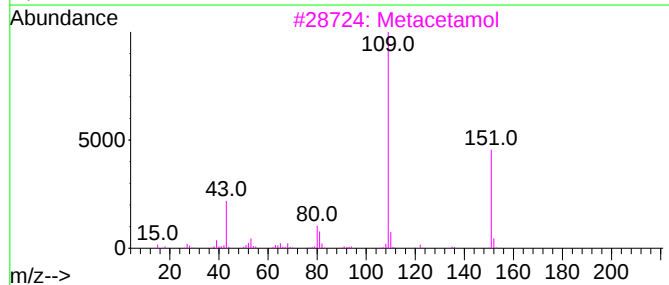
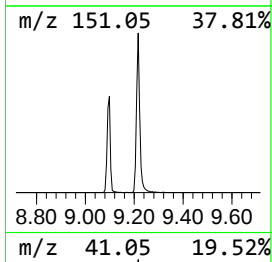
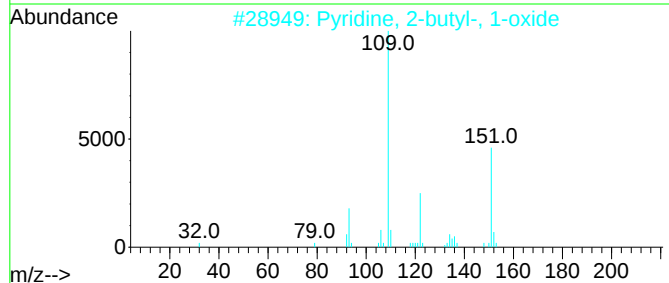
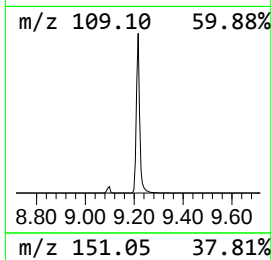
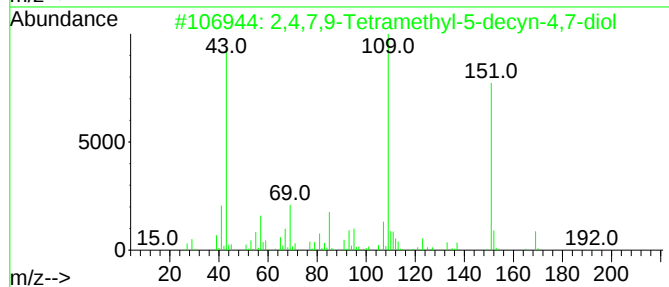
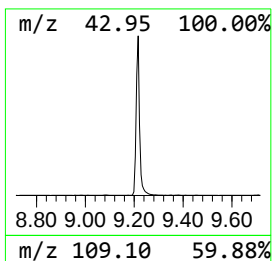
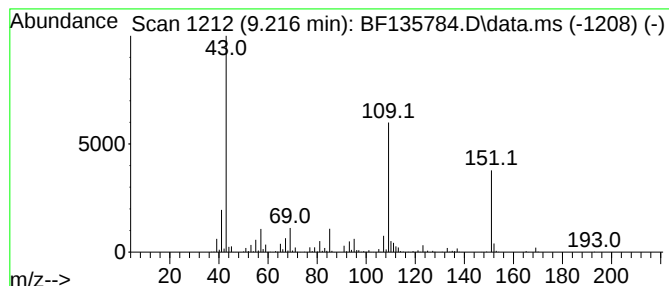
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Peak Number 5 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD			R.T.
9.216	27.95 ng	1111720	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	87
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO		031396-32-4	53
3	Metacetamol	151	C8H9NO2		000621-42-1	49
4	2-Thiophenecarbonitrile	109	C5H3NS		001003-31-2	43
5	4-Amino-2-methylpyrimidine	109	C5H7N3		000074-69-1	38



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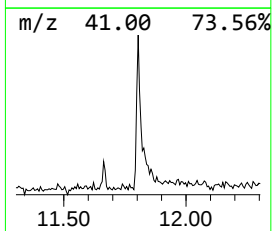
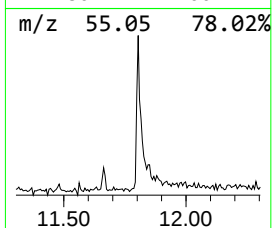
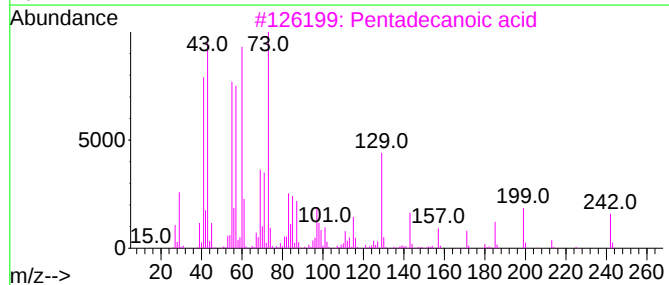
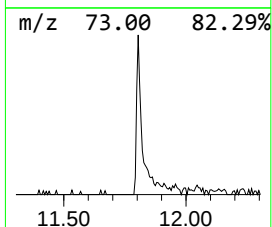
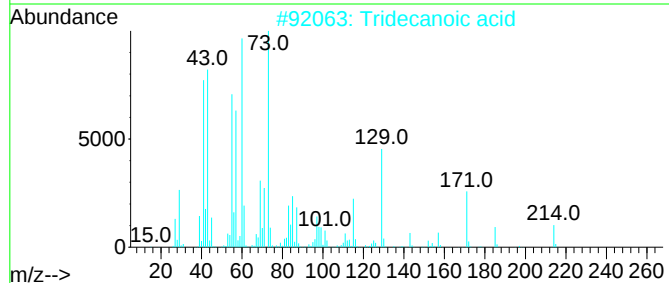
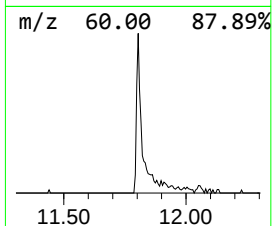
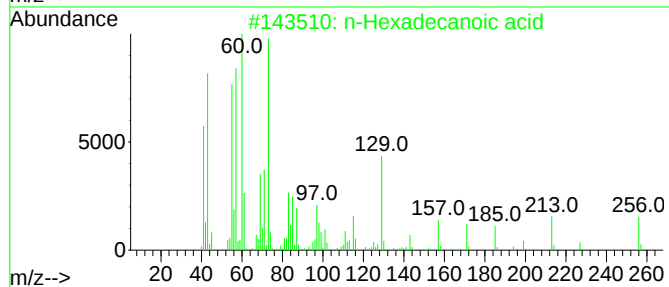
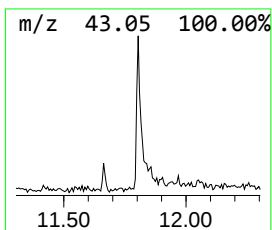
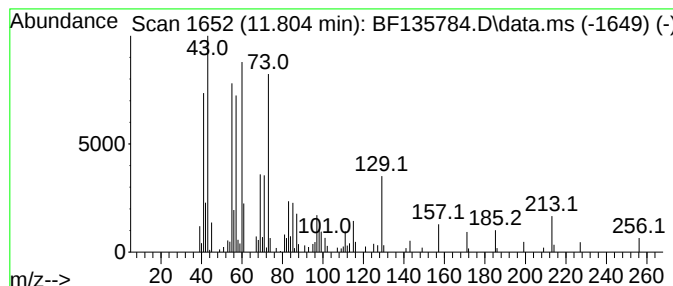
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.804	3.45 ng	147546	Phenanthrene-d10	11.269

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Tridecanoic acid	214	C13H26O2	000638-53-9	76
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	74
4		n-Decanoic acid	172	C10H20O2	000334-48-5	60
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.957	2.8	ng	80491	1	6.734	568152	20.0
Ethanol, 2,2'-o...	6.581	4.4	ng	125361	1	6.734	568152	20.0
2,4,7,9-Tetrame...	9.216	27.9	ng	1111720	3	9.775	795491	20.0
n-Hexadecanoic ...	11.804	3.5	ng	147546	4	11.269	854709	20.0