

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF101822\
 Data File : BF130701.D
 Acq On : 18 Oct 2022 16:44
 Operator : CG\JU
 Sample : N5166-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 5388-1

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-BF101122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130701.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.734	481	484	504	rVB	143038	180411	6.14%	1.152%
2	5.181	557	560	577	rBV	827643	983050	33.45%	6.277%
3	6.228	735	738	758	rBV	529057	588258	20.02%	3.756%
4	6.575	793	797	804	rBV	595577	512071	17.42%	3.270%
5	7.145	890	894	897	rBV	1658006	1588230	54.04%	10.141%
6	7.775	998	1001	1011	rBV	185481	260414	8.86%	1.663%
7	7.857	1011	1015	1023	rVB	781474	672350	22.88%	4.293%
8	8.933	1193	1198	1201	rBV	3532739	2938964	100.00%	18.766%
9	9.057	1215	1219	1228	rVB	79081	80743	2.75%	0.516%
10	9.604	1308	1312	1315	rBV	863026	700579	23.84%	4.473%
11	10.392	1443	1446	1460	rBV	1727656	1485011	50.53%	9.482%
12	11.080	1560	1563	1571	rBV	641619	593617	20.20%	3.790%
13	11.322	1600	1604	1610	rBV	38330	56446	1.92%	0.360%
14	11.486	1628	1632	1635	rBV	59486	46817	1.59%	0.299%
15	11.657	1657	1661	1664	rVB	1377545	1084056	36.89%	6.922%
16	12.186	1749	1751	1757	rVB	82227	78895	2.68%	0.504%
17	12.286	1764	1768	1779	rVB	68551	104762	3.56%	0.669%
18	12.516	1801	1807	1815	rVB	80532	115560	3.93%	0.738%
19	12.668	1829	1833	1836	rBV	1700118	1444575	49.15%	9.224%
20	13.145	1910	1914	1923	rVB	161340	151788	5.16%	0.969%
21	13.710	2004	2010	2013	rBV2	545203	787470	26.79%	5.028%
22	13.739	2013	2015	2025	rVV	226096	246426	8.38%	1.574%
23	13.815	2025	2028	2033	rVB	41578	44952	1.53%	0.287%
24	14.315	2108	2113	2118	rBV	147504	137593	4.68%	0.879%
25	14.715	2177	2181	2183	rBV	99979	102300	3.48%	0.653%
26	14.739	2183	2185	2190	rVB	80699	87852	2.99%	0.561%
27	15.039	2230	2236	2241	rBV	43293	64321	2.19%	0.411%
28	15.092	2241	2245	2256	rVB	450039	523452	17.81%	3.342%

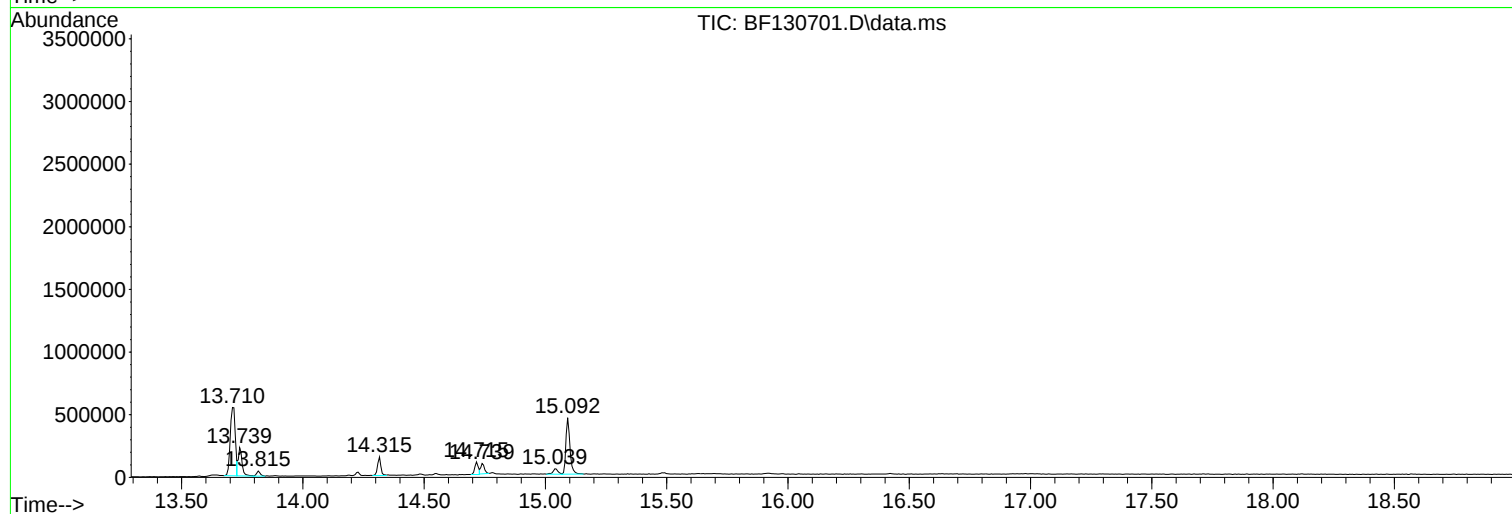
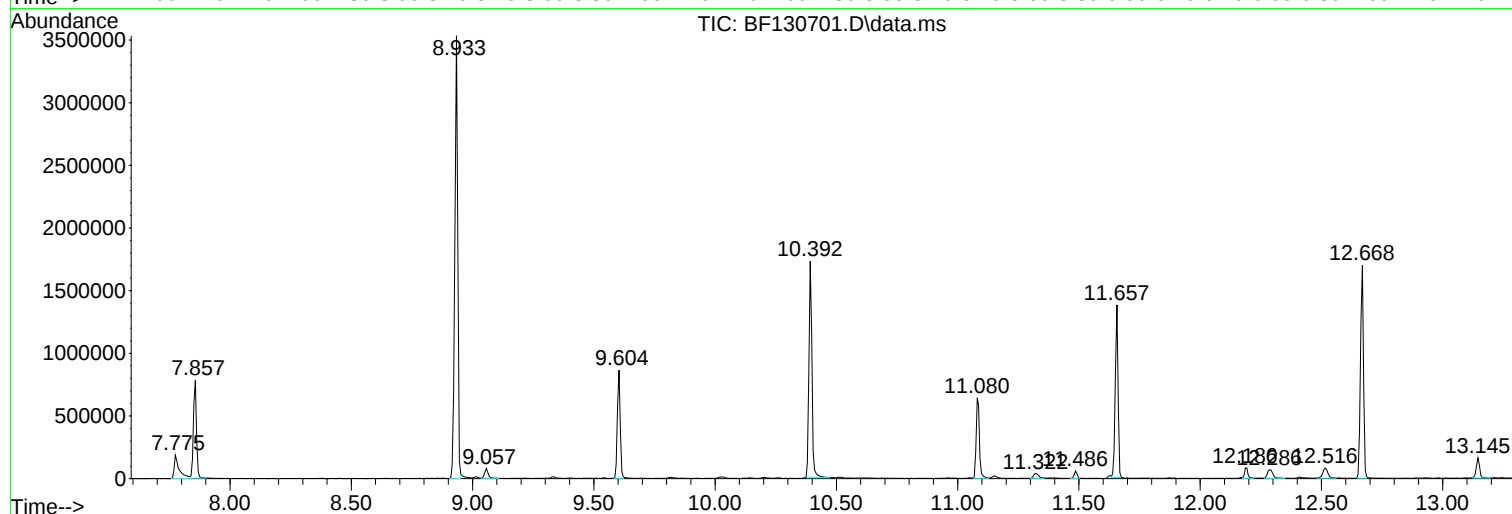
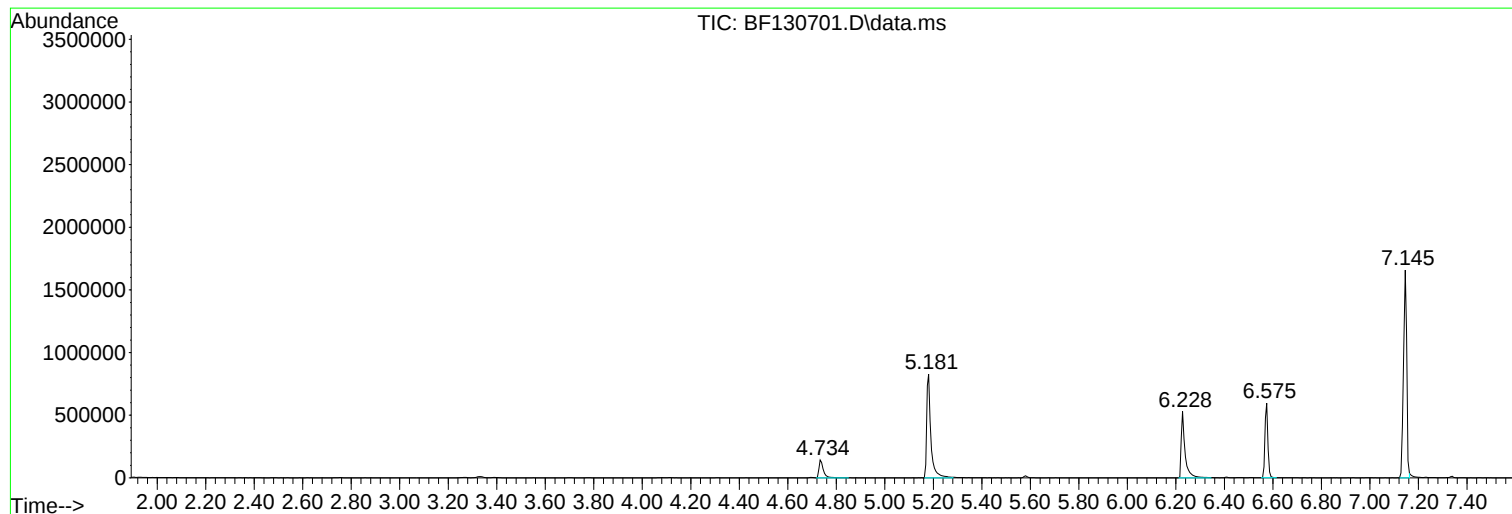
Sum of corrected areas: 15660963

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.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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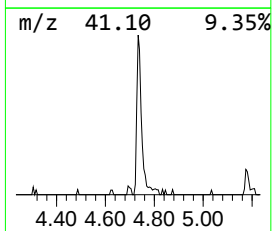
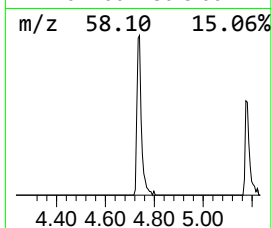
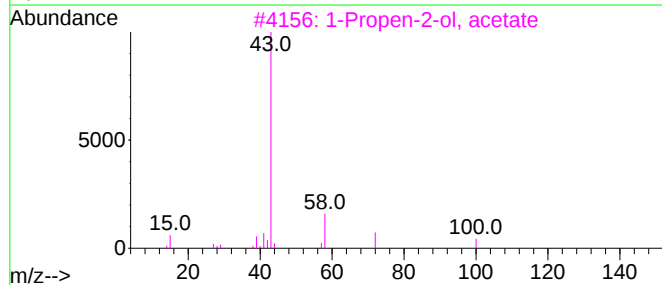
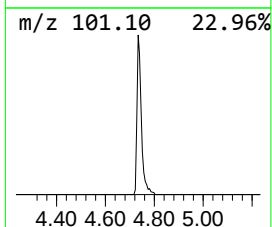
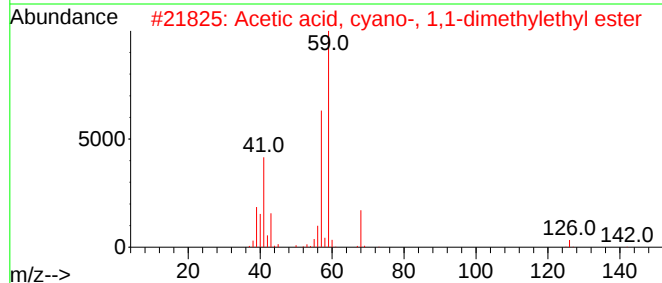
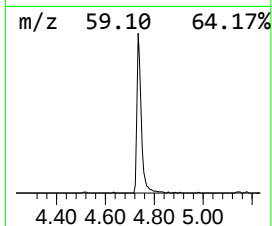
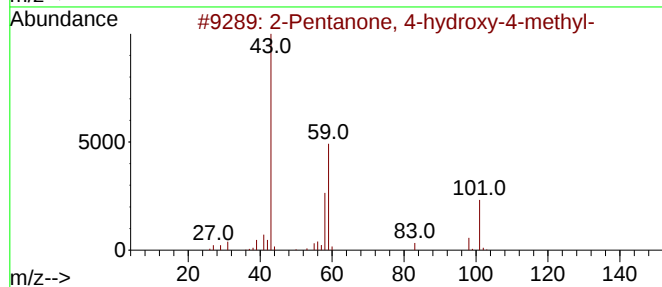
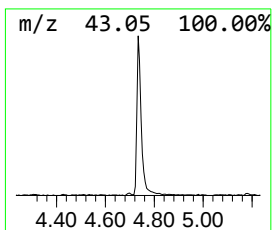
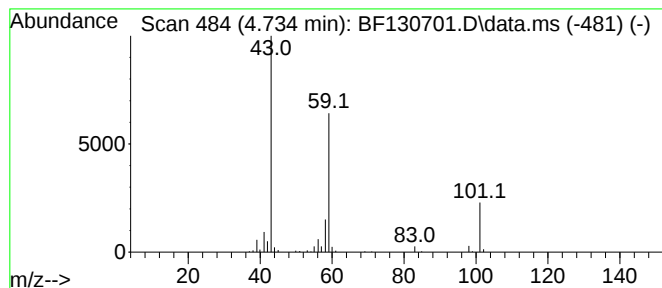
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF101122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.734	7.05 ng	180411	1,4-Dichlorobenzene-d4	6.575

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9		
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9		



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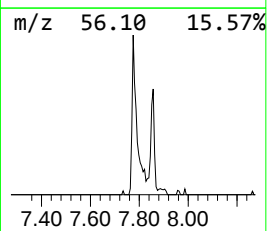
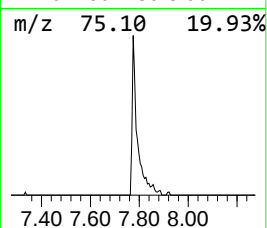
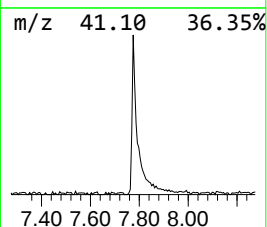
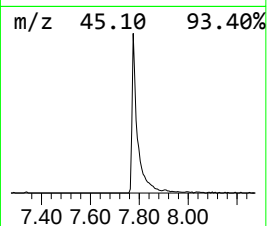
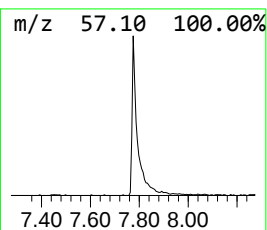
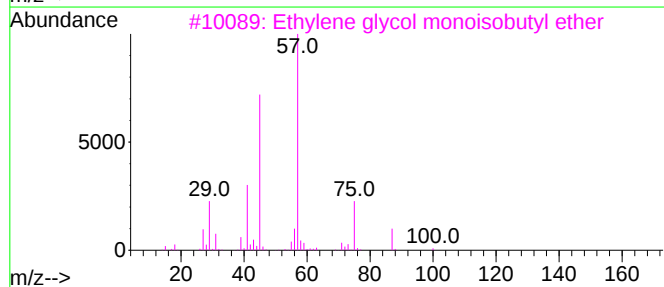
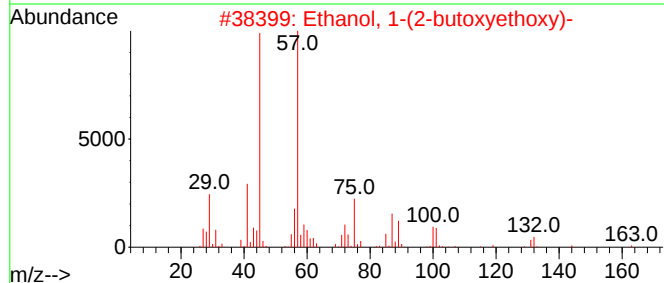
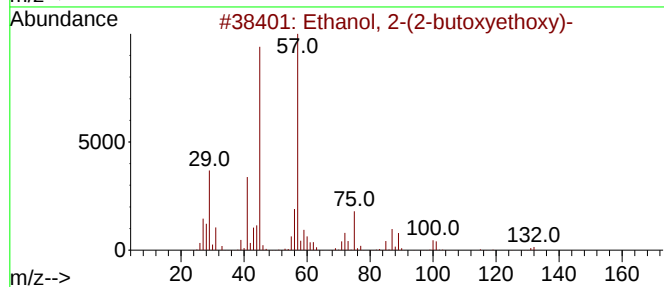
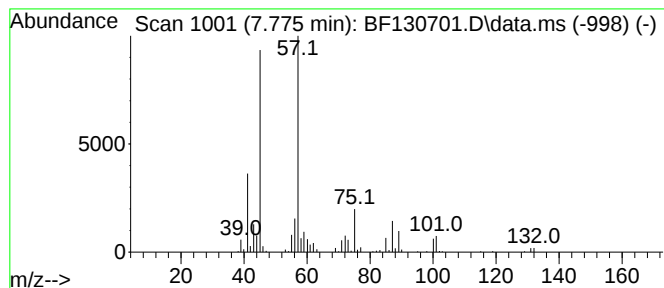
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.775	7.75 ng	260414	Naphthalene-d8	7.857

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			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5			Di-sec-Butyl ether	130	C8H18O	006863-58-7	50



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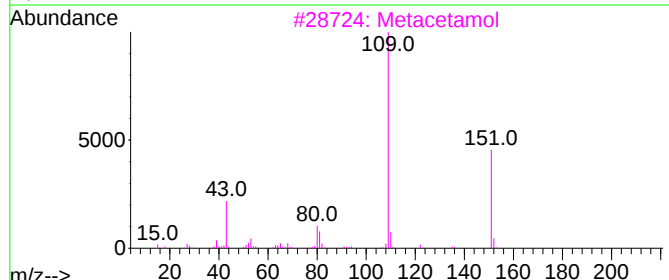
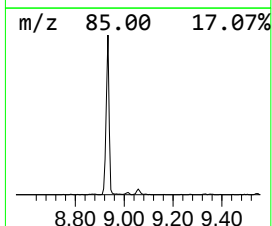
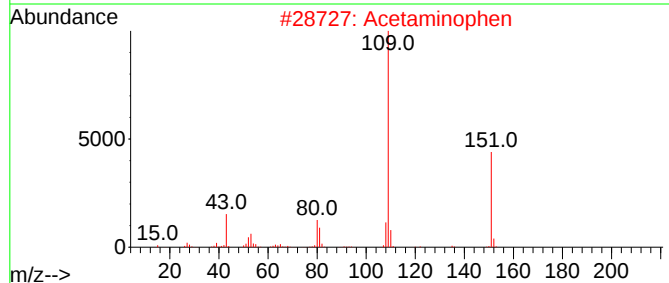
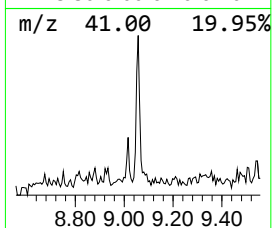
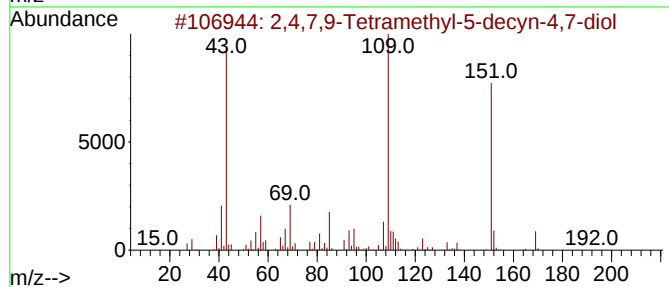
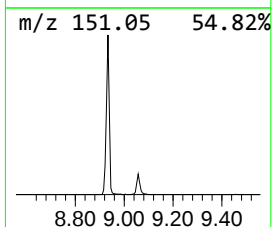
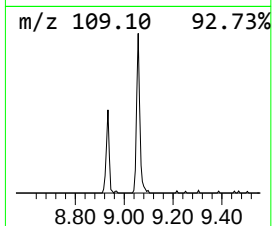
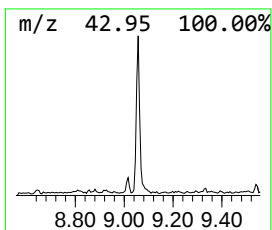
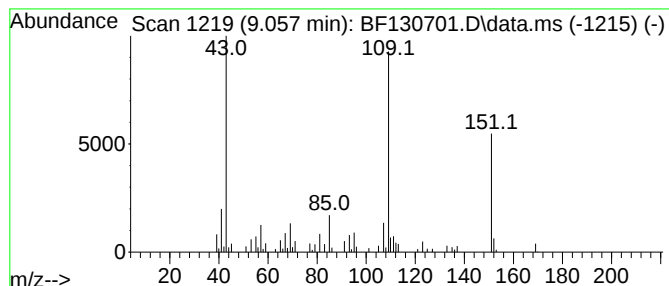
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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.057	2.31 ng	80743	Acenaphthene-d10		9.604

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	Acetaminophen	151	C8H9NO2		000103-90-2	58
3	Metacetamol	151	C8H9NO2		000621-42-1	58
4	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	53
5	2-Fluorobenzyl alcohol, methyl e...	140	C8H9FO		1000365-13-7	43



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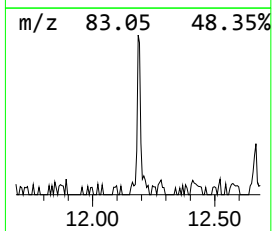
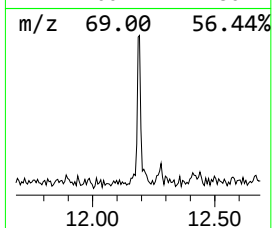
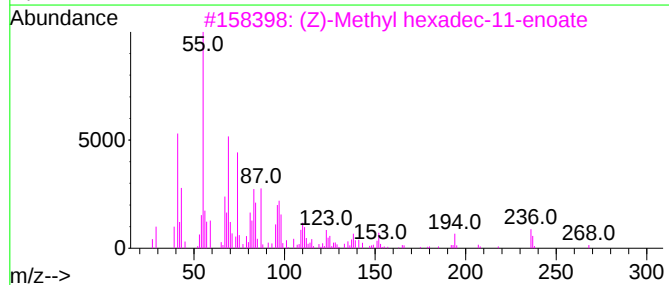
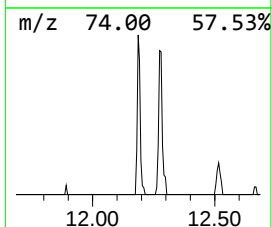
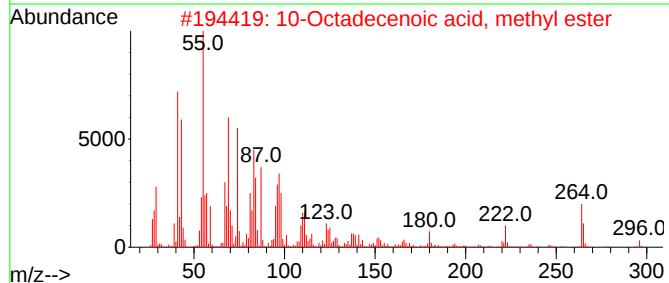
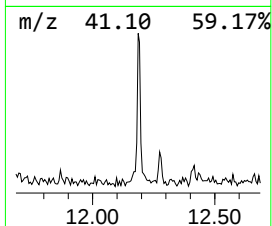
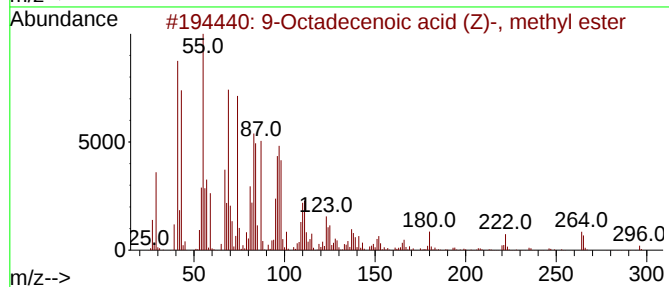
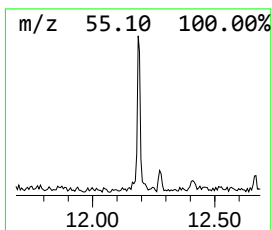
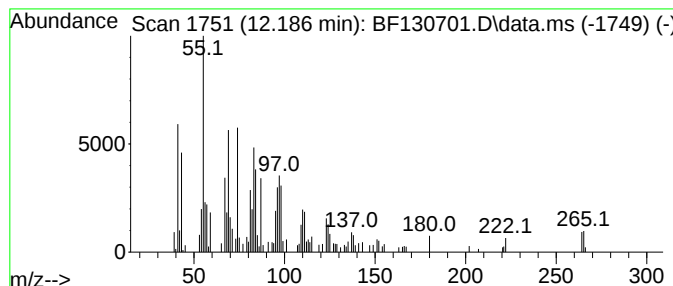
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Peak Number 4 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.186	2.66 ng	78895	Phenanthrene-d10	11.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	95
2			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	94
3			(Z)-Methyl hexadec-11-enoate	268	C17H32O2	000822-05-9	86
4			9-Hexadecenoic acid, methyl este...	268	C17H32O2	001120-25-8	86
5			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.734	7.0	ng	180411	1	6.575	512071	20.0
Ethanol, 2-(2-b...	7.775	7.8	ng	260414	2	7.857	672350	20.0
2,4,7,9-Tetrame...	9.057	2.3	ng	80743	3	9.604	700579	20.0
9-Octadecenoic ...	12.186	2.7	ng	78895	4	11.080	593617	20.0