

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
 Data File : BF135611.D
 Acq On : 05 Oct 2023 21:19
 Operator : CG\JU
 Sample : 04714-04
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135611.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.793	114	120	130	rBV	45194	77485	2.48%	0.341%
2	4.340	379	383	397	rBV	160861	231588	7.43%	1.018%
3	4.969	485	490	507	rBV	1437767	1931048	61.92%	8.490%
4	5.381	556	560	587	rBV	3095838	3118402	100.00%	13.711%
5	5.763	621	625	637	rVB	50640	55204	1.77%	0.243%
6	6.392	728	732	754	rBV	2697307	3034727	97.32%	13.343%
7	6.598	763	767	778	rBV	17583	45396	1.46%	0.200%
8	6.739	787	791	802	rVB	886574	777576	24.94%	3.419%
9	7.304	883	887	890	rBV	2164279	1864642	59.79%	8.198%
10	8.016	1004	1008	1023	rBV	1182002	986959	31.65%	4.339%
11	9.092	1187	1191	1195	rBV	3398367	3023951	96.97%	13.295%
12	9.210	1207	1211	1221	rVB	222107	226672	7.27%	0.997%
13	9.769	1303	1306	1310	rBV	1065034	937546	30.06%	4.122%
14	10.569	1438	1442	1459	rBV	1523226	1519311	48.72%	6.680%
15	11.263	1557	1560	1568	rBV	847295	745327	23.90%	3.277%
16	11.798	1648	1651	1663	rBV2	100680	163596	5.25%	0.719%
17	12.592	1784	1786	1794	rBV6	19929	40716	1.31%	0.179%
18	12.857	1827	1831	1835	rBV	2148727	2108059	67.60%	9.269%
19	13.821	1988	1995	2003	rBV8	36729	124090	3.98%	0.546%
20	13.921	2009	2012	2023	rVB	758893	748858	24.01%	3.293%
21	14.698	2141	2144	2148	rVB3	29332	32588	1.05%	0.143%
22	15.027	2197	2200	2206	rVB	62252	72121	2.31%	0.317%
23	15.392	2257	2262	2273	rBV	589964	809749	25.97%	3.560%
24	15.833	2334	2337	2344	rVB	43864	68618	2.20%	0.302%

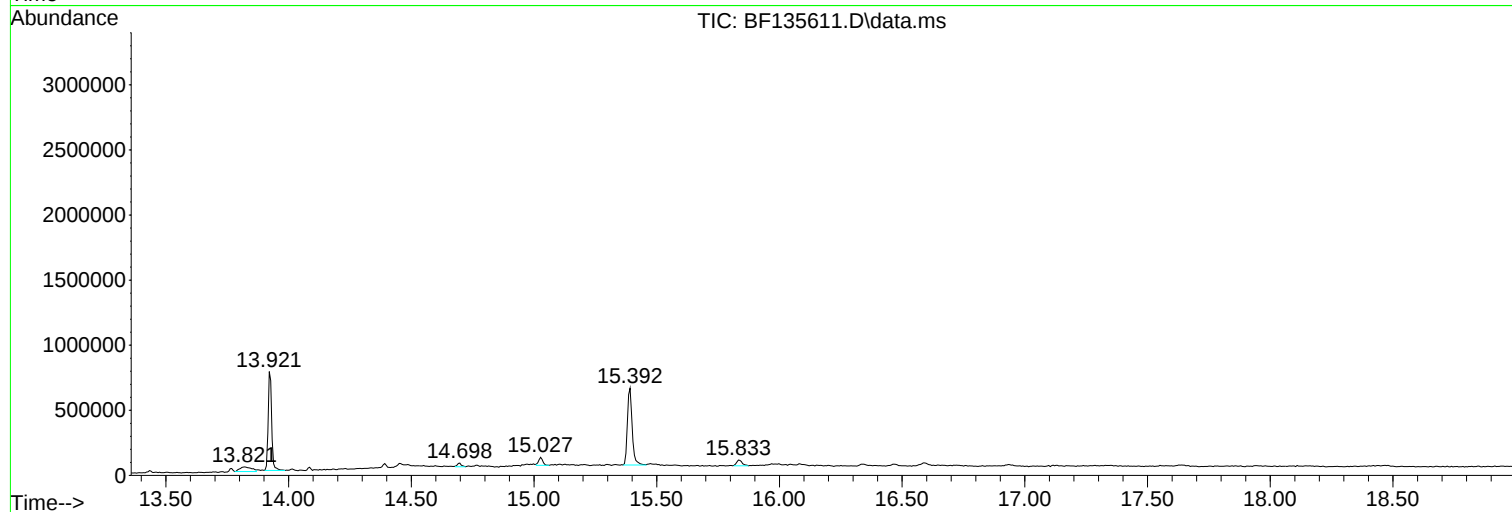
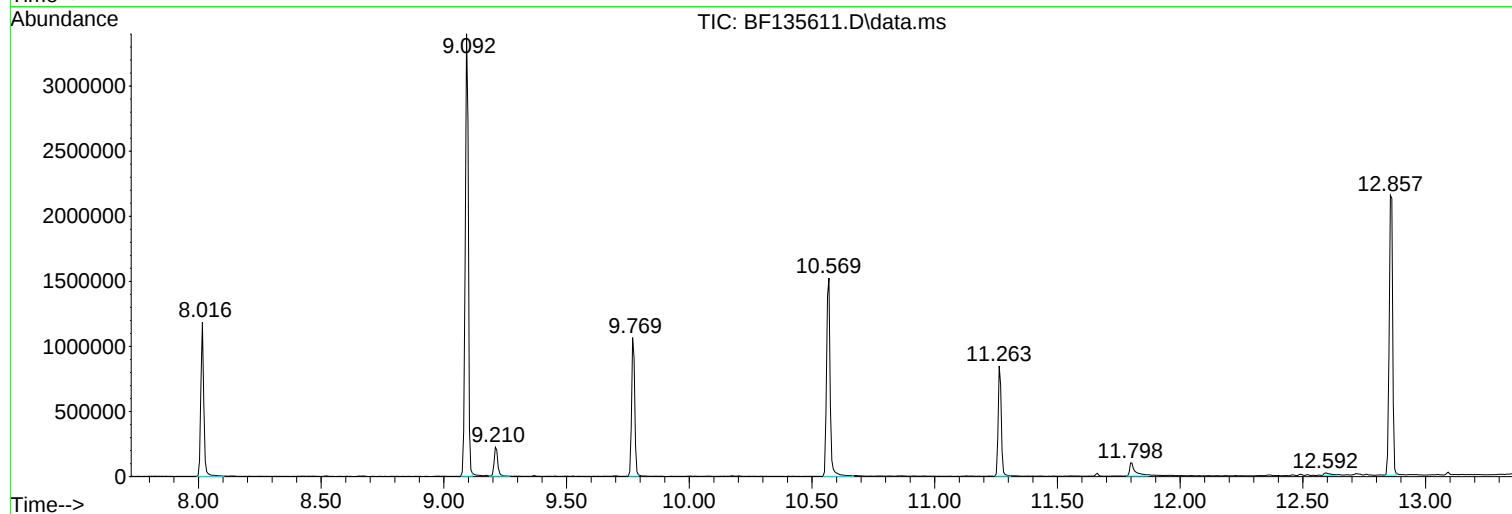
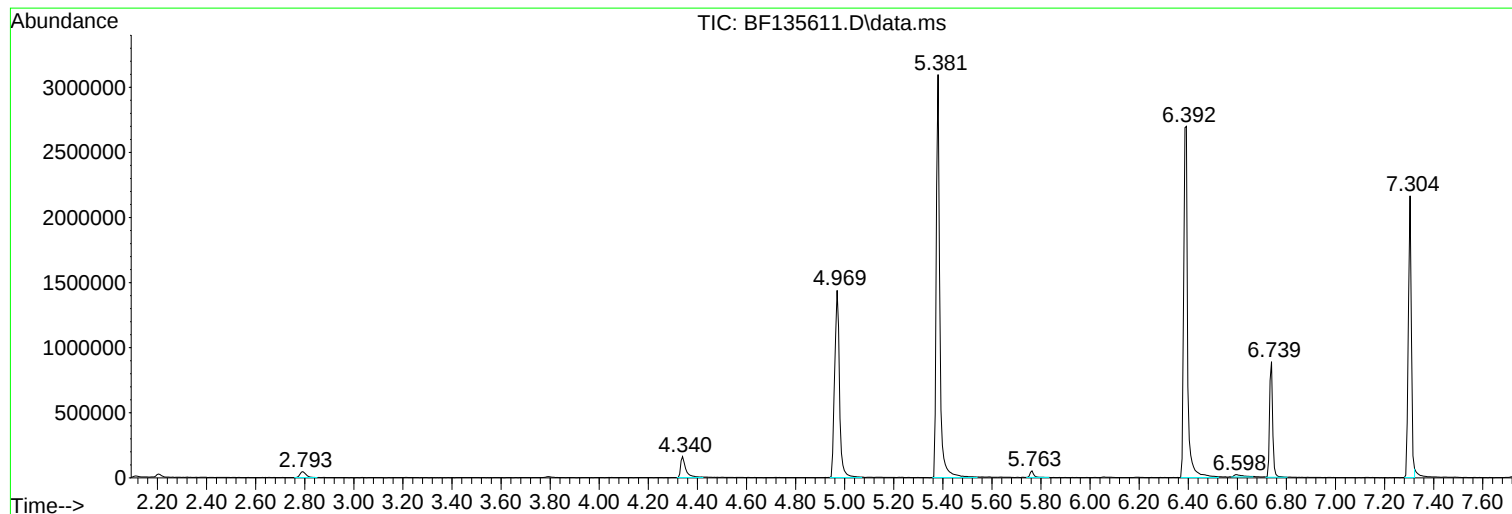
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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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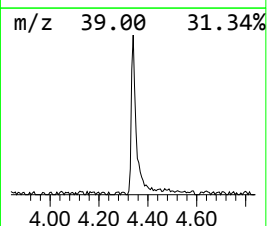
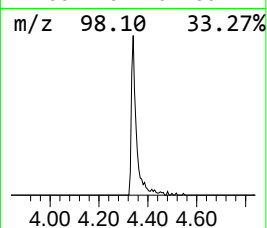
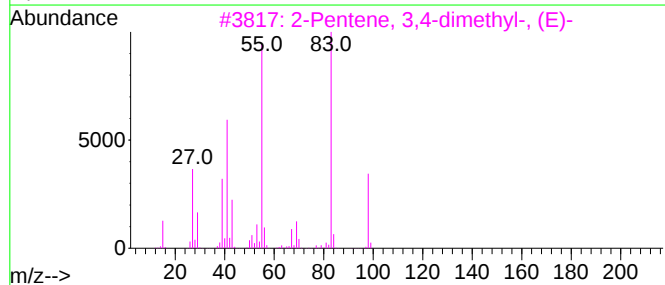
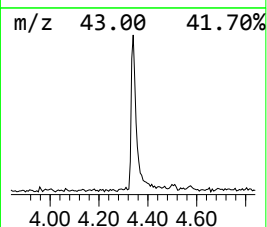
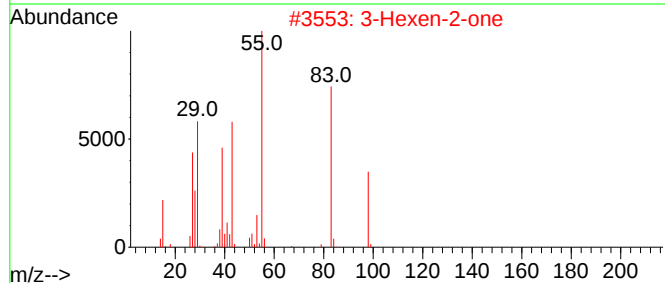
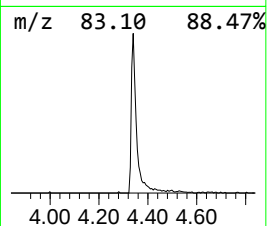
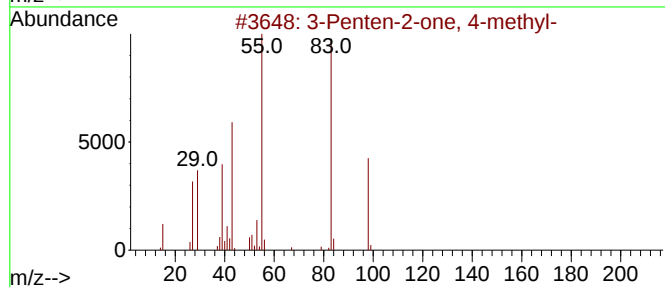
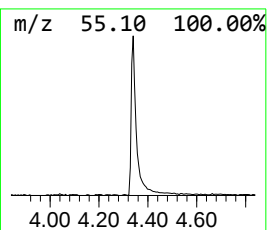
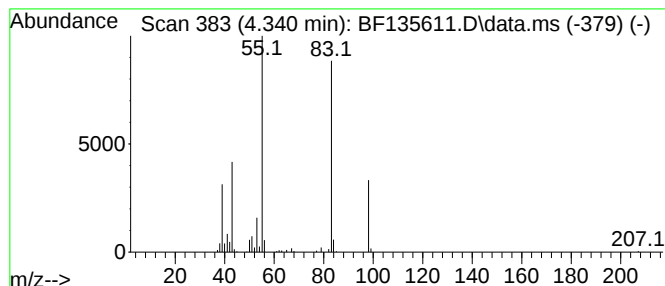
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.340	5.96 ng	231588	1,4-Dichlorobenzene-d4	6.739

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	78
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5			2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	72



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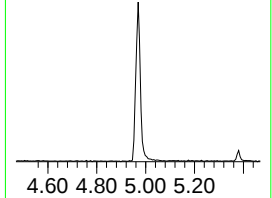
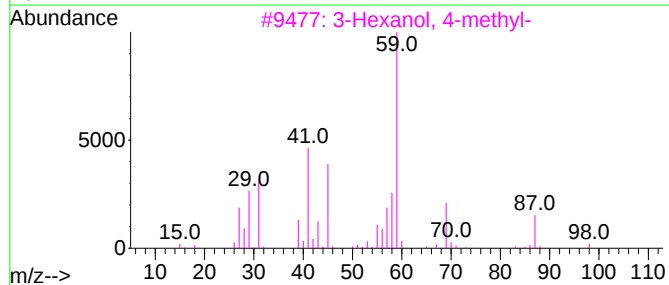
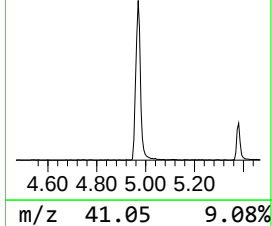
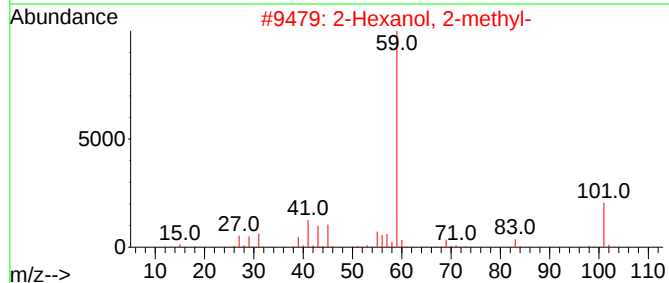
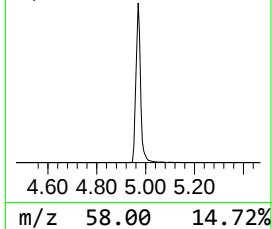
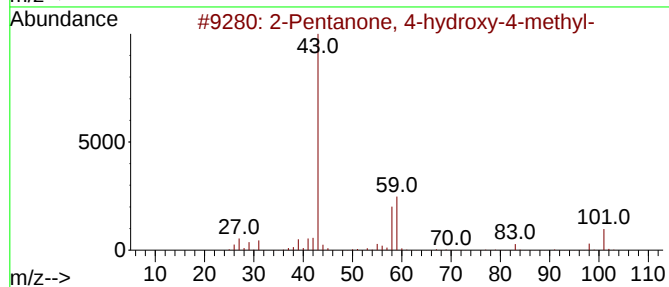
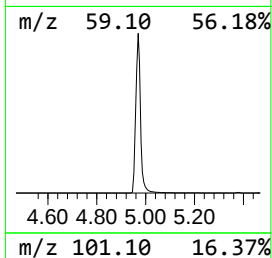
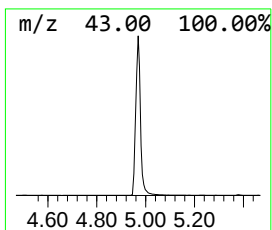
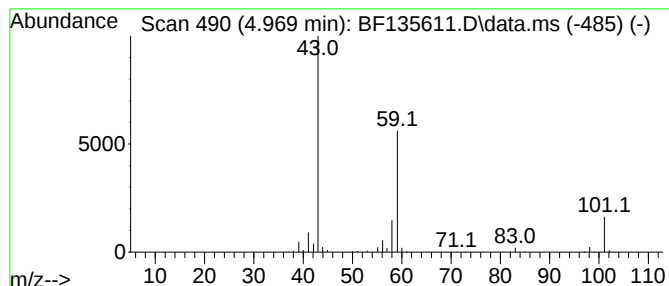
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.969	49.67 ng	1931050	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	59		
2	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		



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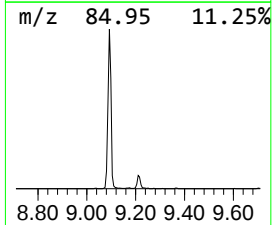
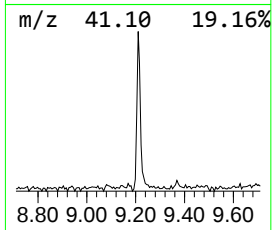
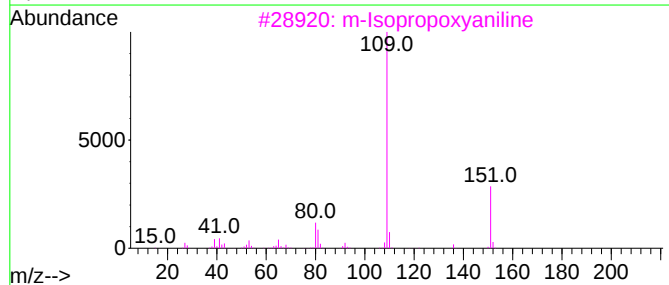
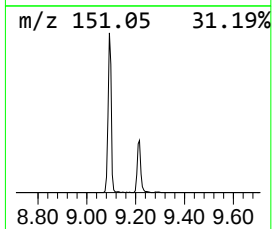
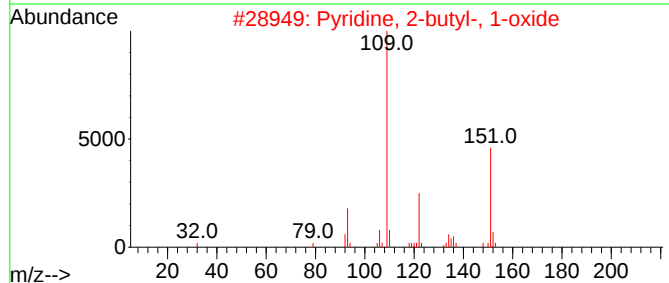
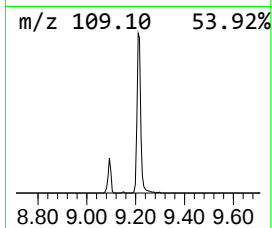
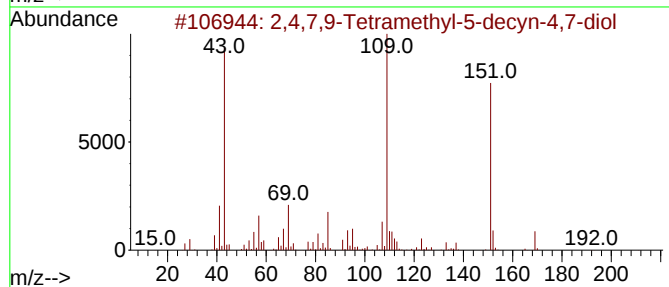
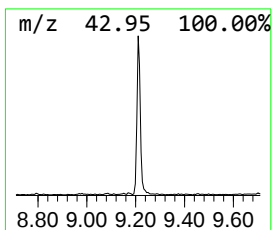
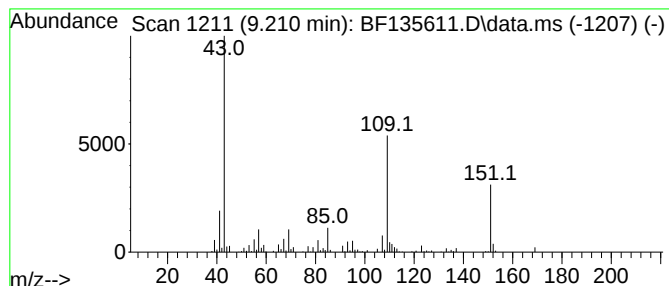
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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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.
9.210	4.84 ng	226672	Acenaphthene-d10			9.769

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	m-Isopropoxyaniline	151	C9H13NO	041406-00-2	47	
4	2-Thiophenecarbonitrile	109	C5H3NS	001003-31-2	47	
5	Metacetamol	151	C8H9NO2	000621-42-1	47	



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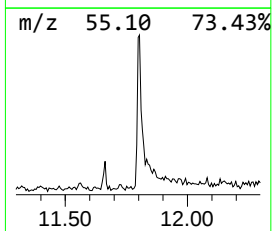
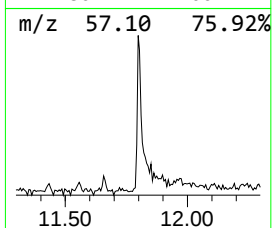
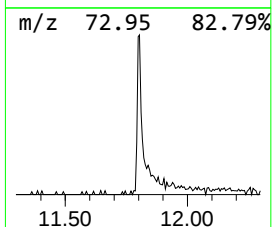
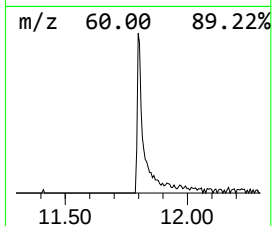
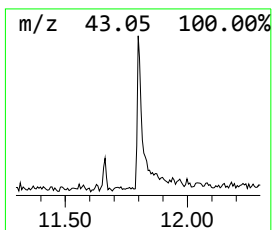
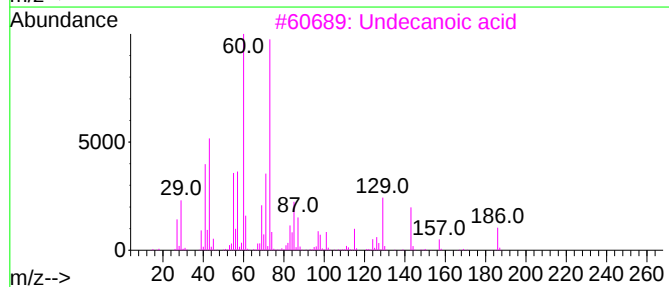
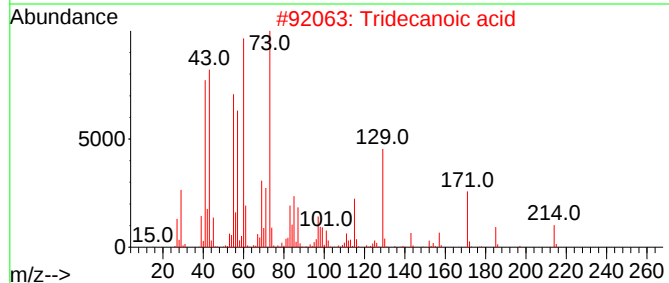
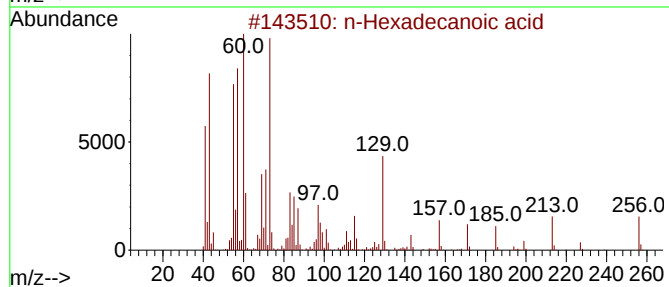
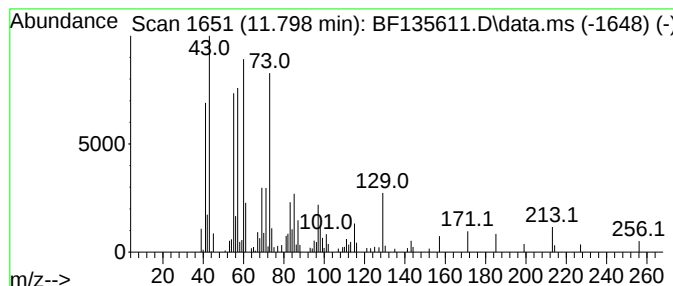
Instrument :
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.798	4.39 ng	163596	Phenanthrene-d10	11.263	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	81
3	Undecanoic acid	186	C11H22O2	000112-37-8	72
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	72



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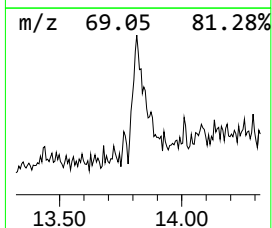
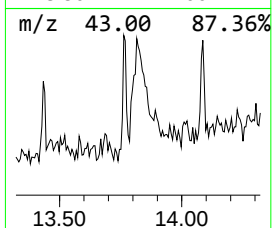
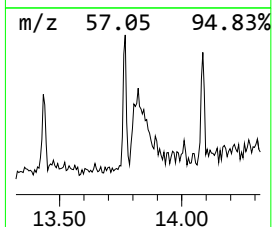
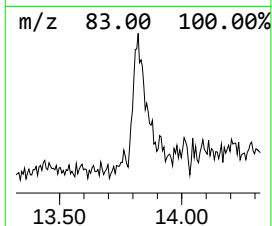
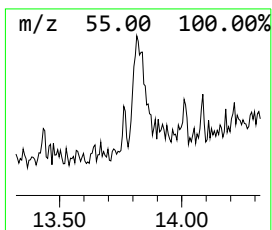
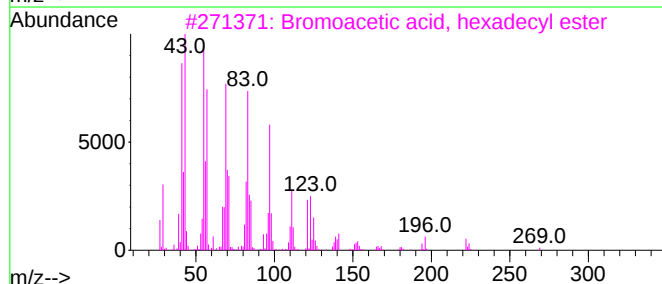
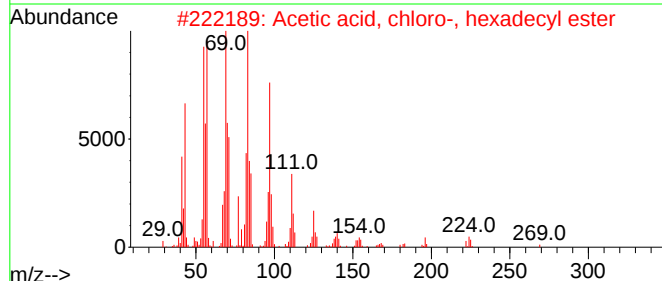
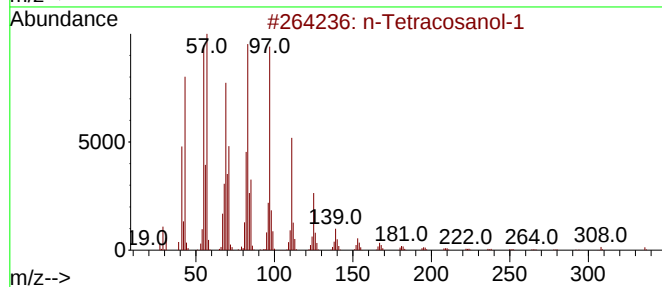
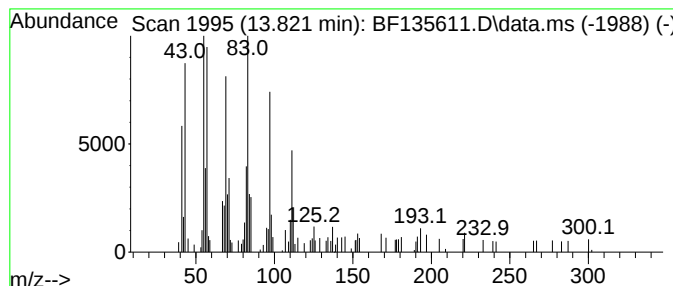
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Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.821	3.31 ng	124090	Chrysene-d12	13.921	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	90
2	Acetic acid, chloro-, hexadecyl ...	318	C18H35ClO2	052132-58-8	87
3	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	86
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	64
5	Cyclopropane, nonyl-	168	C12H24	074663-85-7	52



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.340	6.0	ng	231588	1	6.739	777576	20.0
2-Pentanone, 4-...	4.969	49.7	ng	1931050	1	6.739	777576	20.0
2,4,7,9-Tetrame...	9.210	4.8	ng	226672	3	9.769	937546	20.0
n-Hexadecanoic ...	11.798	4.4	ng	163596	4	11.263	745327	20.0
n-Tetracosanol-1	13.821	3.3	ng	124090	5	13.921	748858	20.0