

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
 Data File : BF133072.D
 Acq On : 26 Apr 2023 19:01
 Operator : CG\JU
 Sample : 02491-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S2S-TP3

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133072.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.287	365	374	380	rBV	129351	162455	2.45%	0.379%
2	4.934	478	484	501	rVB	1358881	1935955	29.23%	4.519%
3	5.351	550	555	558	rBV	4844455	5504532	83.11%	12.850%
4	5.745	618	622	626	rVB	86254	75281	1.14%	0.176%
5	6.381	723	730	732	rBV	4693071	5776950	87.23%	13.486%
6	6.734	786	790	793	rBV	1301107	989123	14.93%	2.309%
7	7.304	881	887	889	rBV	3650294	3742469	56.51%	8.736%
8	8.016	1005	1008	1012	rBV	1656817	1359846	20.53%	3.174%
9	9.098	1187	1192	1195	rBV	6722673	6188481	93.44%	14.446%
10	9.769	1302	1306	1309	rBV	2035209	1570716	23.72%	3.667%
11	10.480	1424	1427	1431	rBV	275853	235437	3.55%	0.550%
12	10.557	1435	1440	1443	rBV	3957117	3972833	59.99%	9.274%
13	11.251	1554	1558	1561	rBV	1929002	1653354	24.96%	3.860%
14	11.786	1645	1649	1653	rBV2	246991	235146	3.55%	0.549%
15	12.457	1760	1763	1766	rBV	112412	95179	1.44%	0.222%
16	12.568	1777	1782	1790	rBV5	45788	73591	1.11%	0.172%
17	12.686	1796	1802	1805	rVB	100721	101735	1.54%	0.237%
18	12.845	1823	1829	1832	rBV	6343831	6622880	100.00%	15.460%
19	13.804	1985	1992	1994	rBV4	54094	112822	1.70%	0.263%
20	13.880	2001	2005	2009	rBV	1281635	1224541	18.49%	2.859%
21	14.898	2173	2178	2187	rBV	55667	107323	1.62%	0.251%
22	15.304	2242	2247	2253	rBV	880691	1020906	15.41%	2.383%
23	16.668	2474	2479	2486	rVB3	35384	76006	1.15%	0.177%

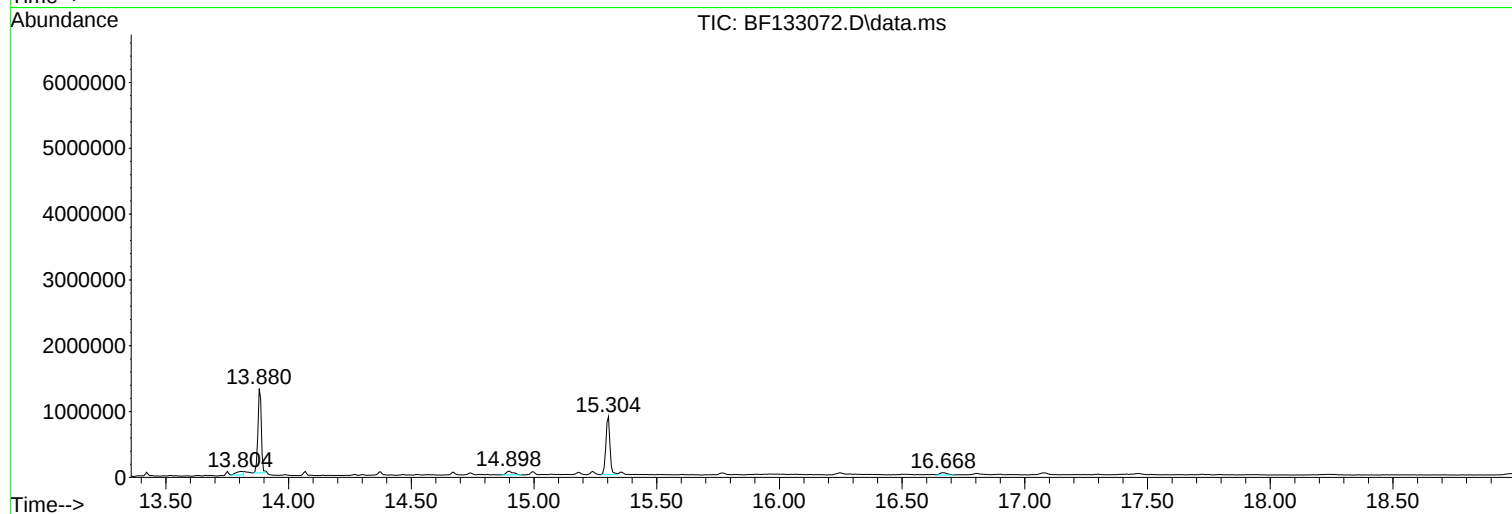
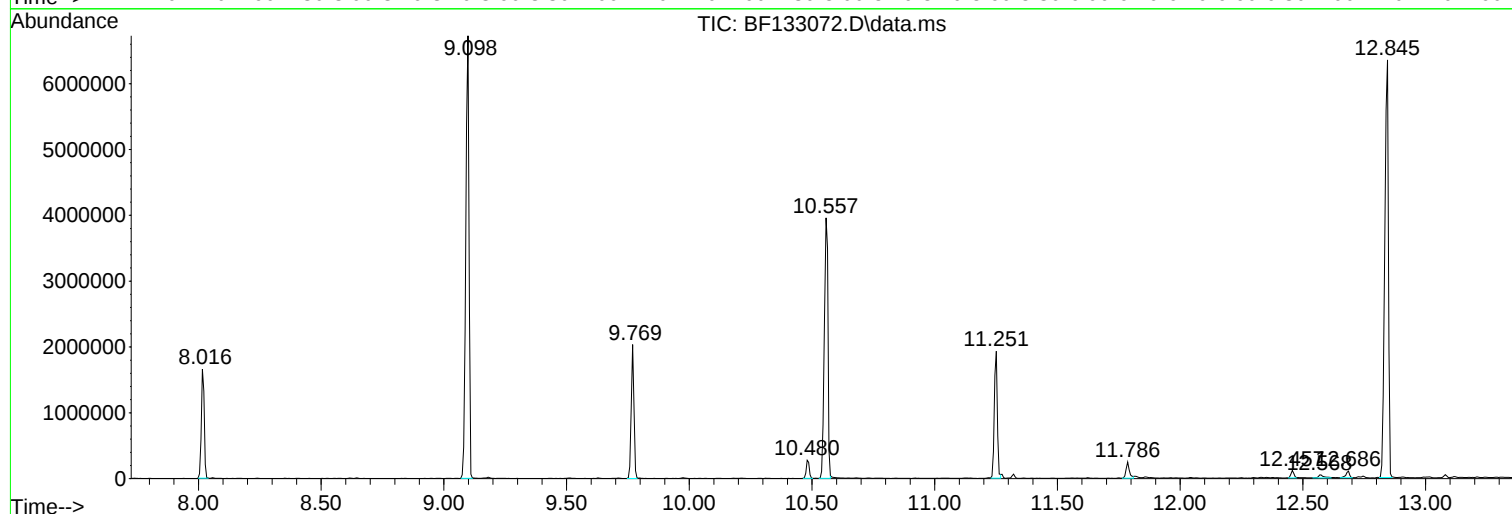
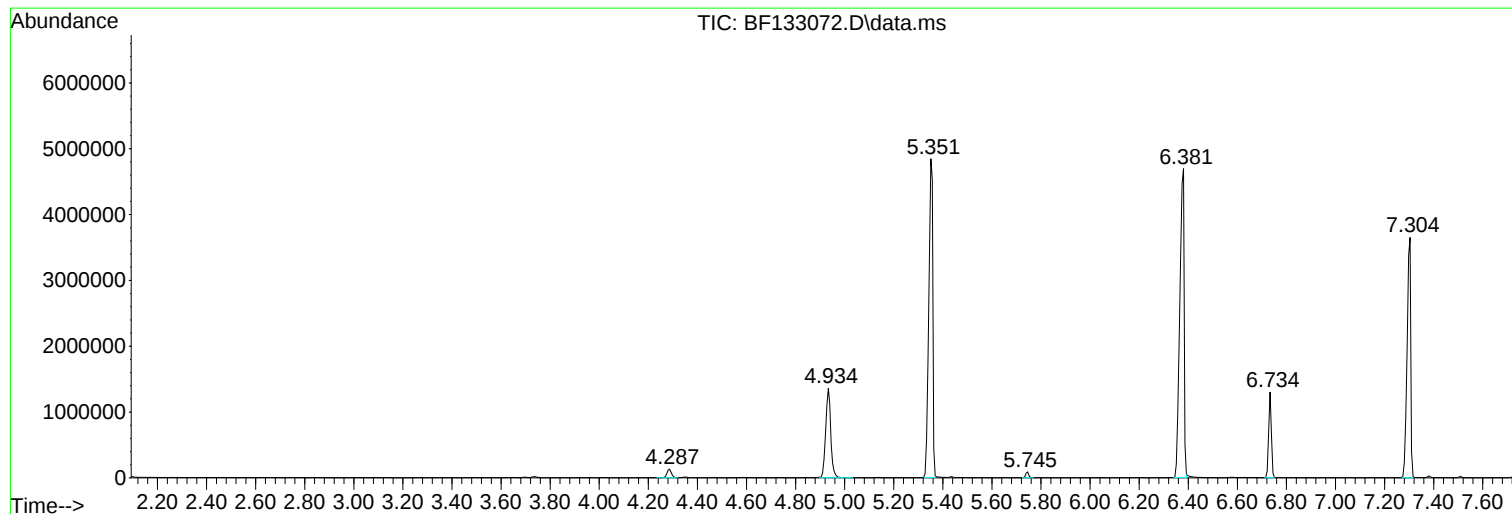
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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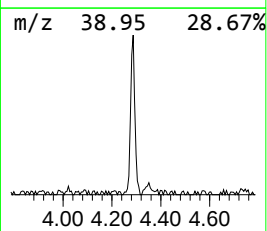
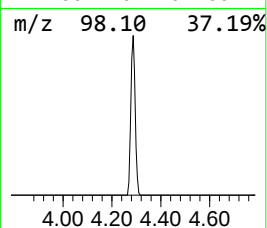
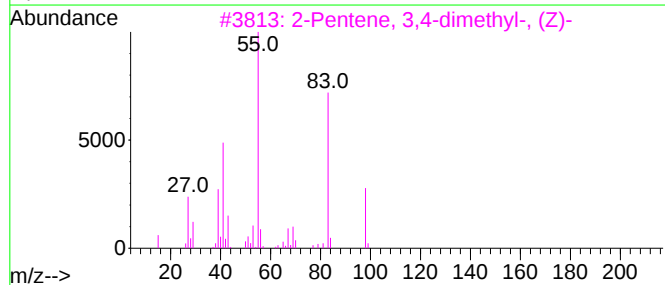
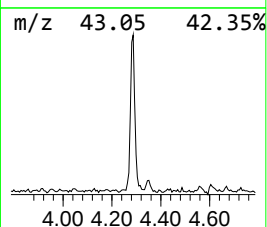
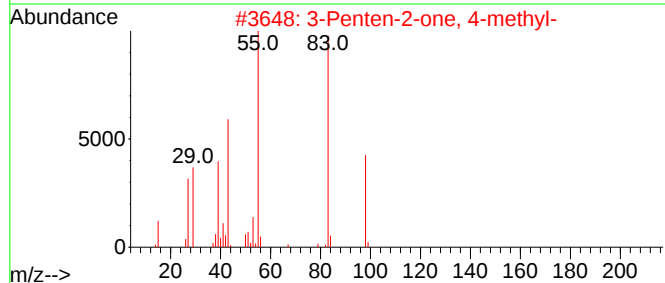
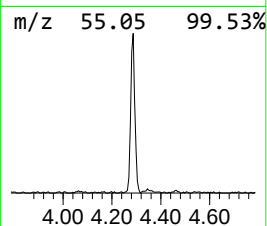
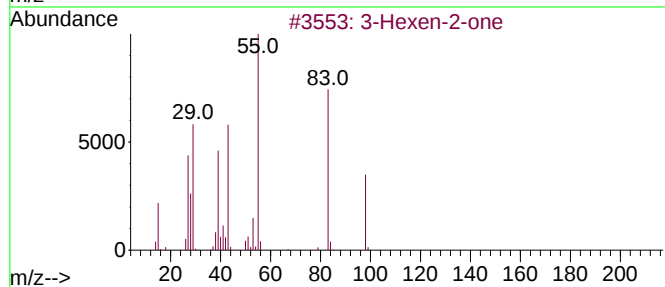
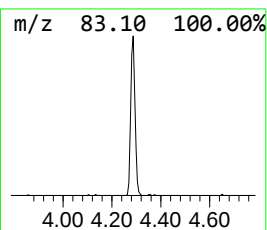
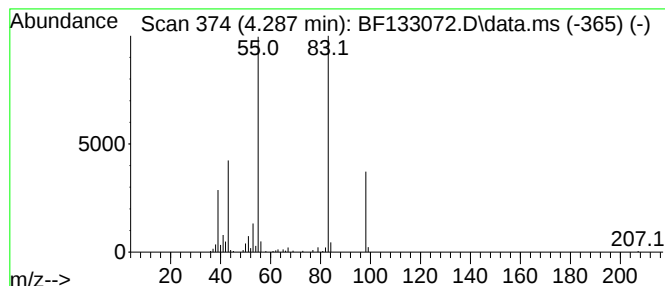
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 3-Hexen-2-one Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.287	3.28 ng	162455	1,4-Dichlorobenzene-d4	6.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hexen-2-one	98	C6H10O	000763-93-9	91
2			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
3			2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
4			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
5			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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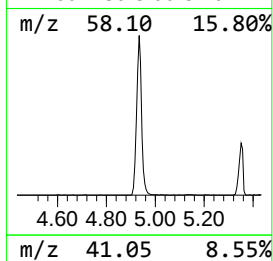
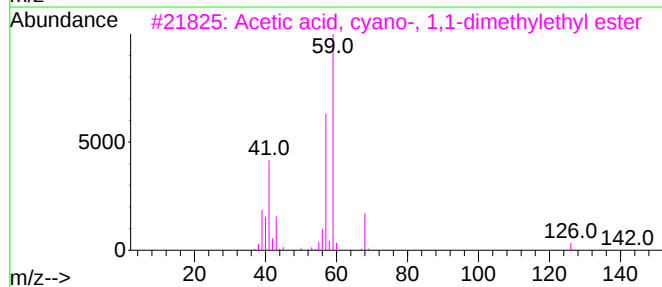
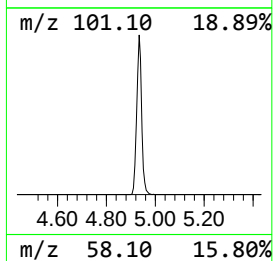
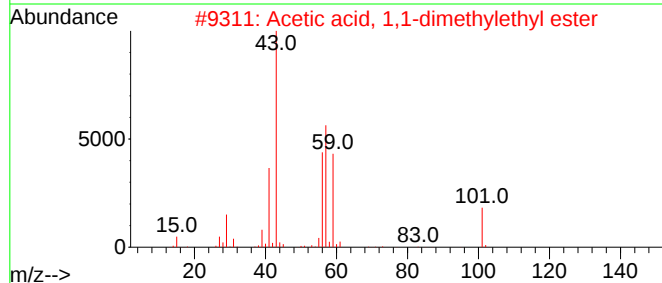
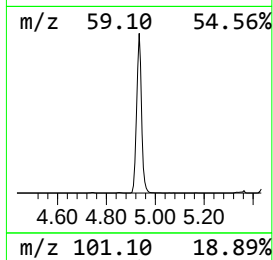
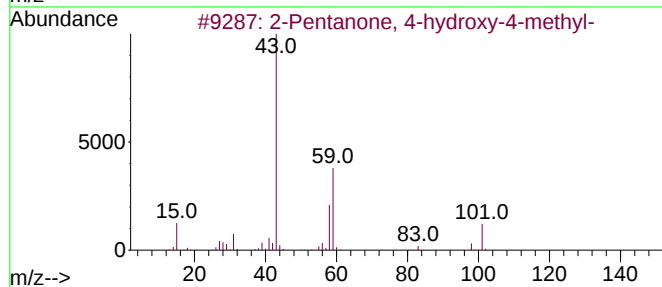
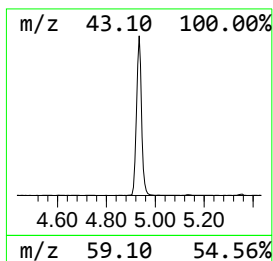
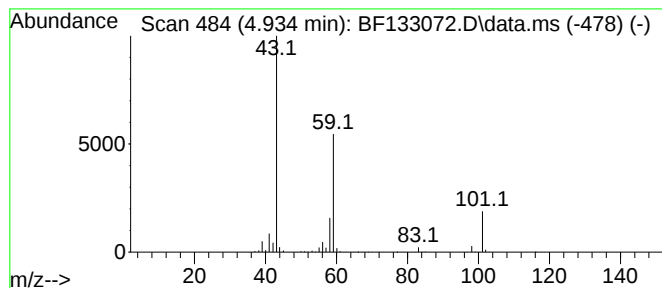
Instrument :
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ClientSampleId :
S2S-TP3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.934	39.14 ng	1935960	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	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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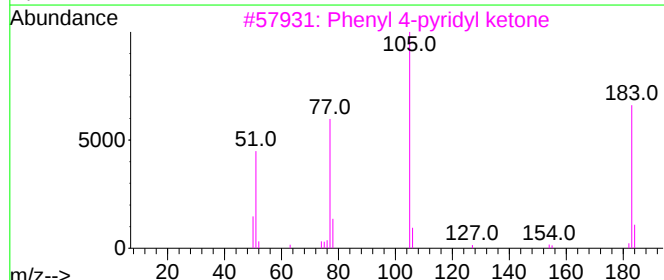
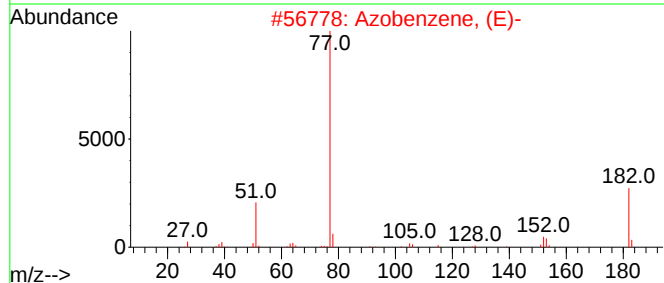
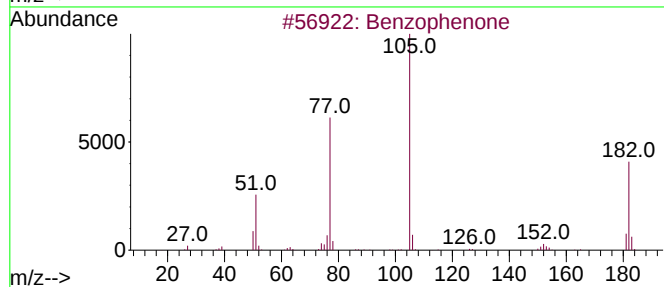
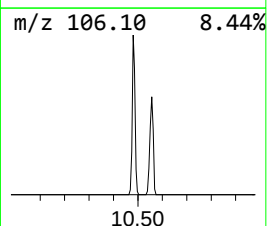
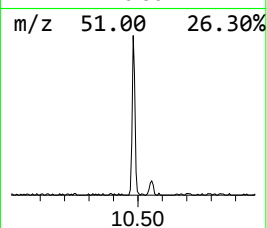
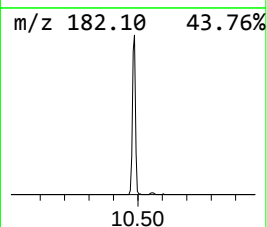
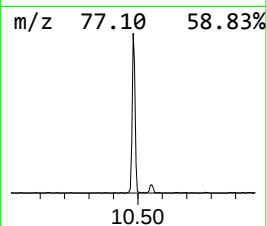
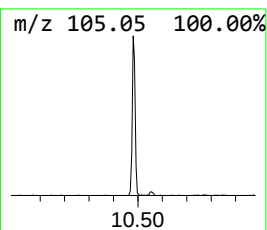
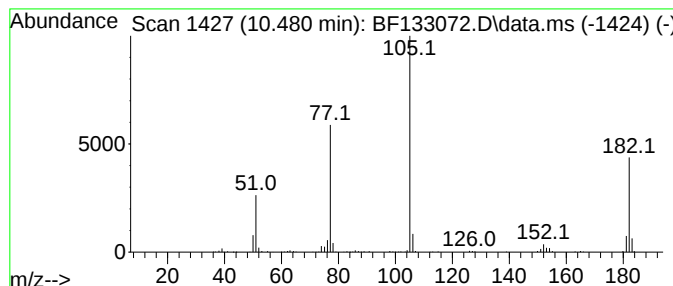
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Peak Number 3 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	3.00 ng	235437	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Azobenzene, (E)-	182	C12H10N2	017082-12-1	50
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	50
4			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	47
5			Methyl hippurate, N-trifluoroace...	289	C12H10F3NO4	073749-76-5	47



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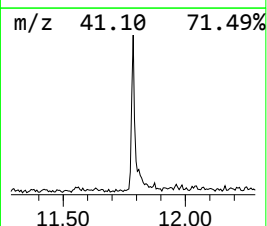
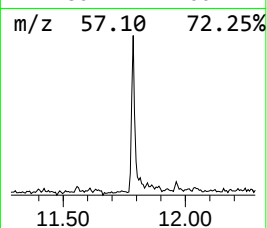
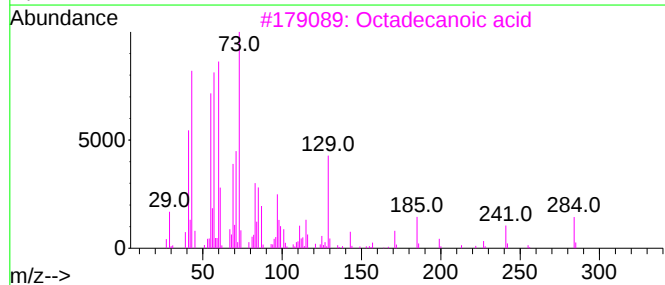
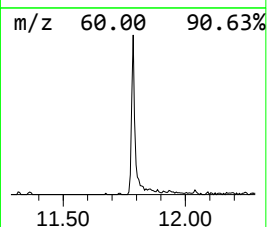
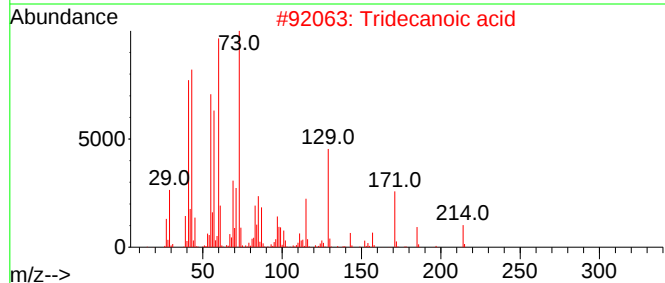
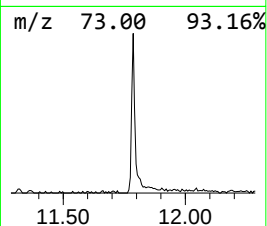
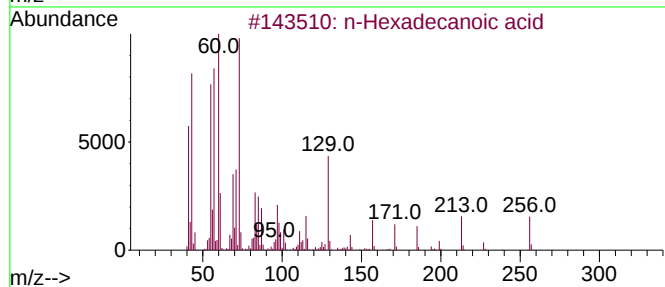
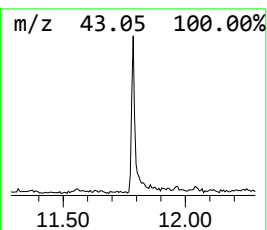
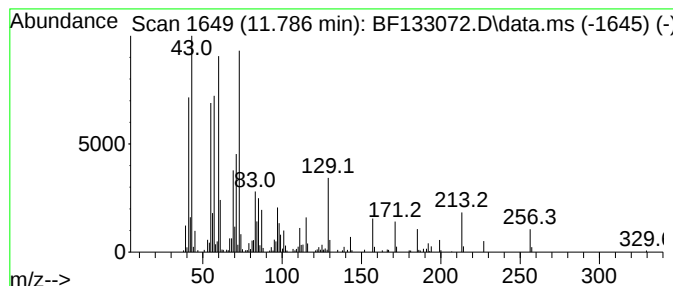
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	2.84 ng	235146	Phenanthrene-d10	11.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	80



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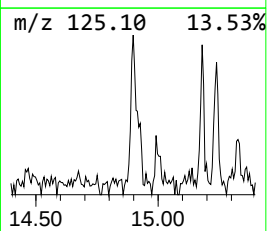
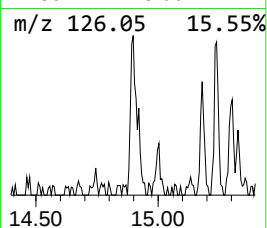
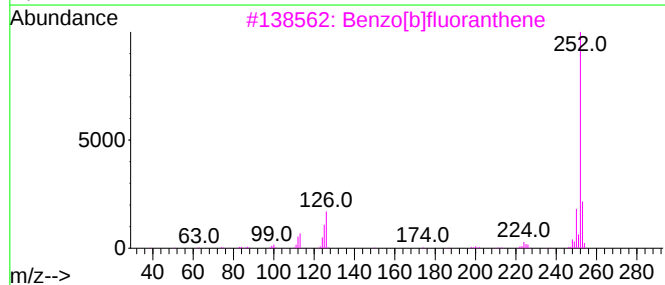
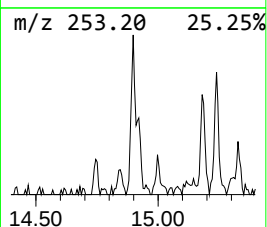
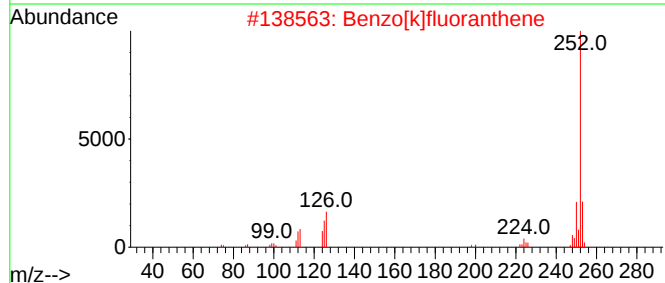
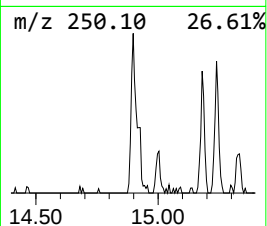
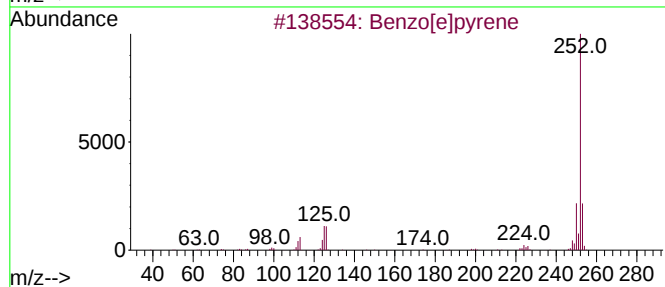
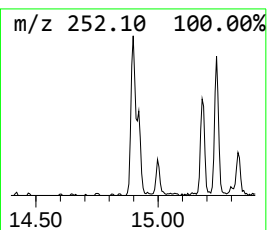
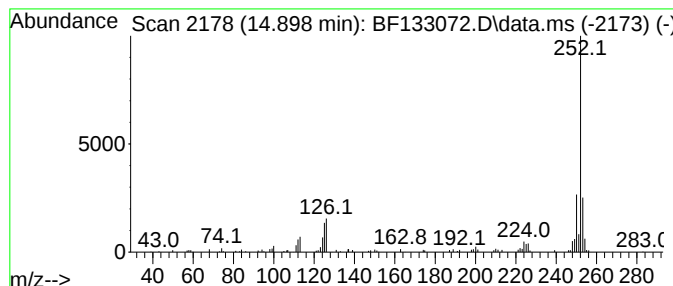
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Benzo[e]pyrene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.898	2.10 ng	107323	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	98
2			Benzo[k]fluoranthene	252	C20H12	000207-08-9	98
3			Benzo[b]fluoranthene	252	C20H12	000205-99-2	97
4			Benzo[a]pyrene	252	C20H12	000050-32-8	95
5			Benzo[j]fluoranthene	252	C20H12	000205-82-3	95



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Hexen-2-one	4.287	3.3	ng	162455	1	6.734	989123	20.0
2-Pentanone, 4-...	4.934	39.1	ng	1935960	1	6.734	989123	20.0
Benzophenone	10.480	3.0	ng	235437	3	9.769	1570720	20.0
n-Hexadecanoic ...	11.786	2.8	ng	235146	4	11.251	1653350	20.0
Benzo[e]pyrene	14.898	2.1	ng	107323	6	15.304	1020910	20.0