

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122223\
 Data File : BF136694.D
 Acq On : 22 Dec 2023 19:43
 Operator : CG\JU
 Sample : 05796-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RT-SB-06-13-14

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136694.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.016	494	498	504	rVB	59481	65166	3.93%	0.713%
2	5.428	563	568	571	rBV	1277058	1242626	74.86%	13.599%
3	6.434	734	739	741	rBV	1450404	1504903	90.66%	16.470%
4	6.781	795	798	802	rBV	428983	379085	22.84%	4.149%
5	7.346	889	894	897	rBV	1173446	1040156	62.66%	11.383%
6	7.698	952	954	963	rBV	74571	82090	4.95%	0.898%
7	8.057	1012	1015	1019	rVB	500554	440631	26.55%	4.822%
8	8.604	1104	1108	1112	rBV3	31327	42020	2.53%	0.460%
9	9.140	1195	1199	1202	rBV	2095661	1659914	100.00%	18.166%
10	9.257	1216	1219	1222	rBV	55333	48525	2.92%	0.531%
11	9.816	1311	1314	1318	rVB	499319	392971	23.67%	4.301%
12	10.610	1445	1449	1452	rBV	548821	475113	28.62%	5.200%
13	11.310	1564	1568	1571	rBV	404459	357000	21.51%	3.907%
14	11.845	1657	1659	1663	rBV2	124488	125556	7.56%	1.374%
15	12.916	1837	1841	1843	rBV	1356722	1281736	77.22%	14.027%

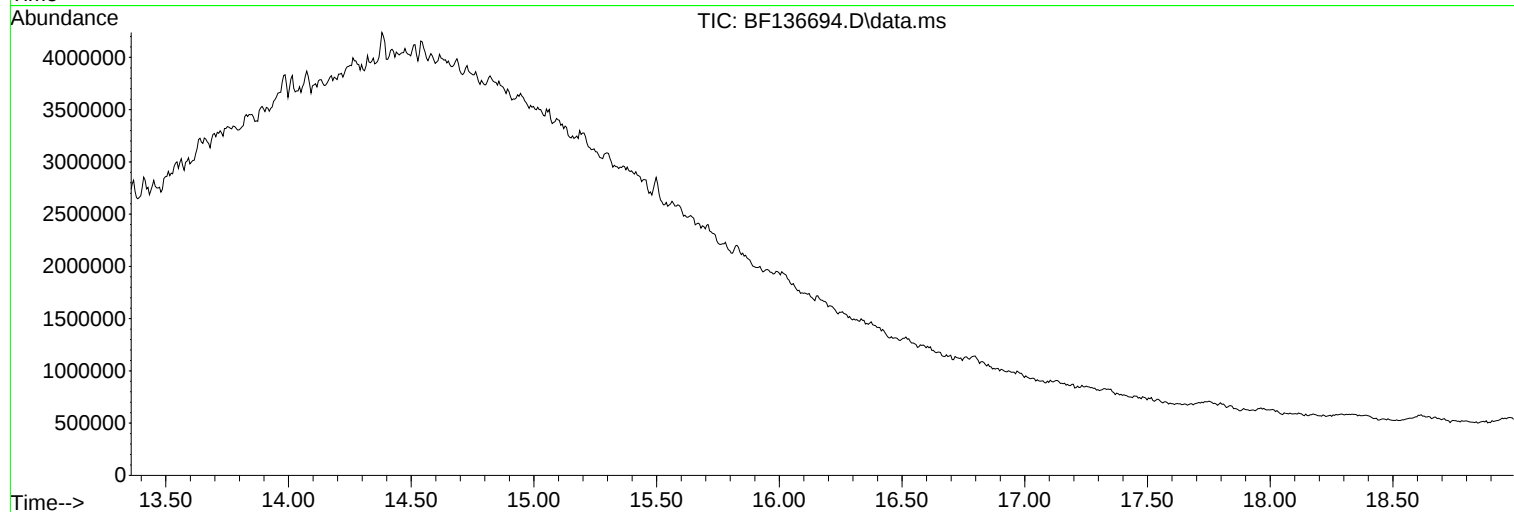
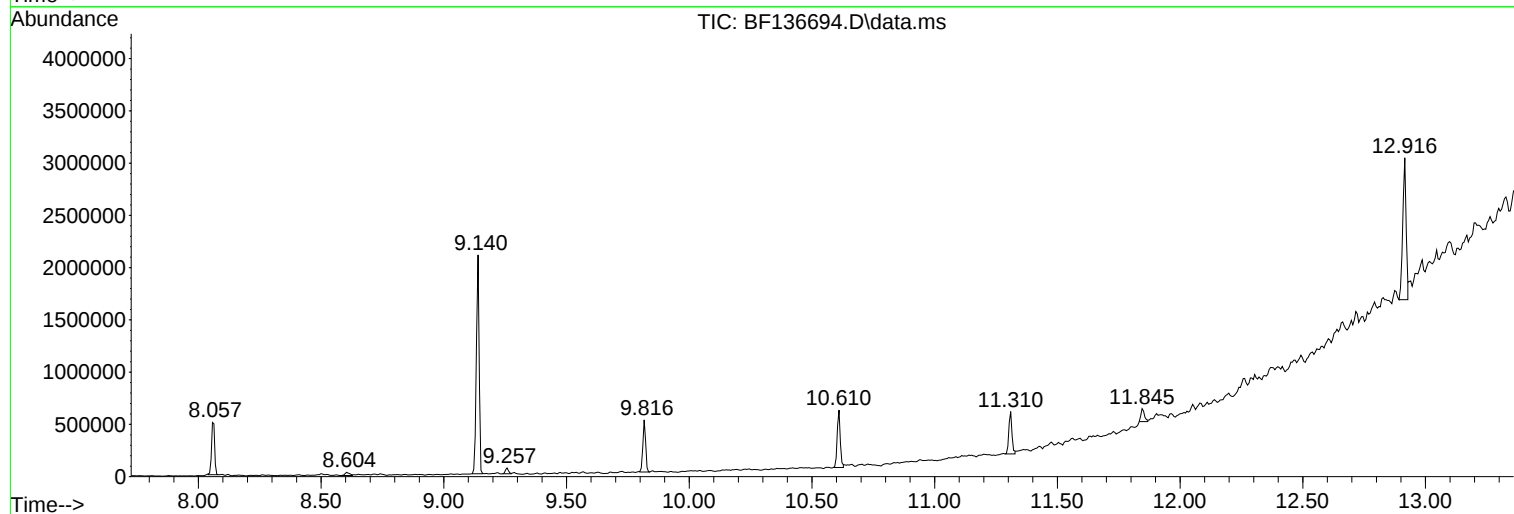
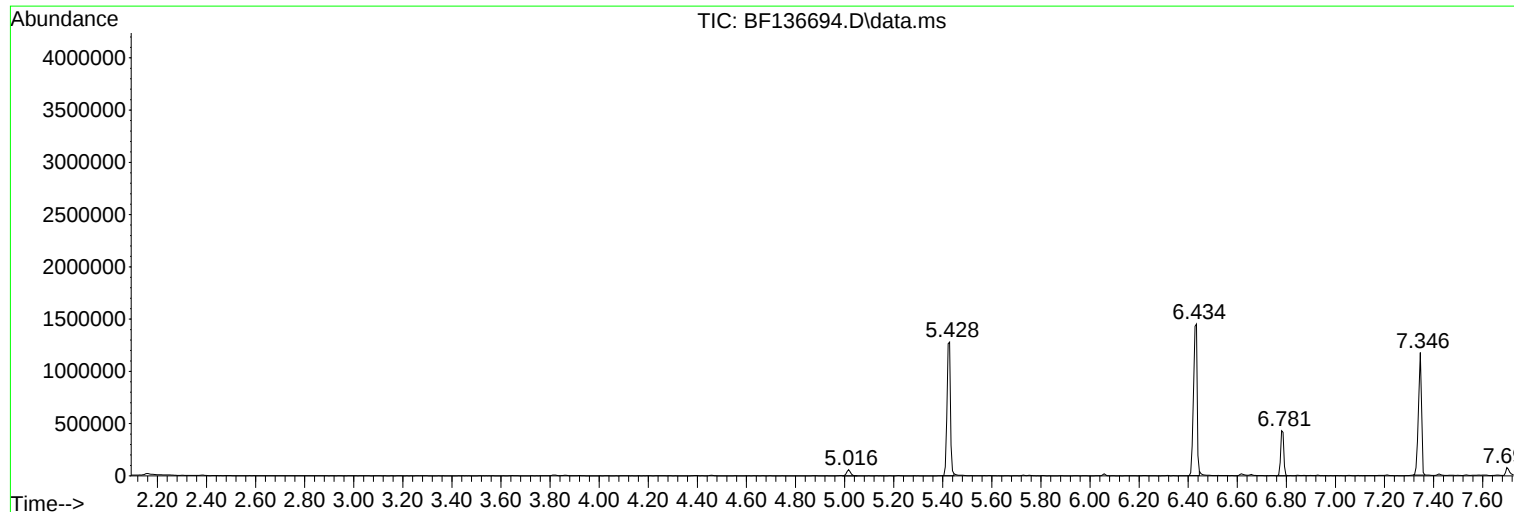
Sum of corrected areas: 9137492

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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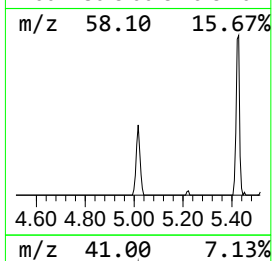
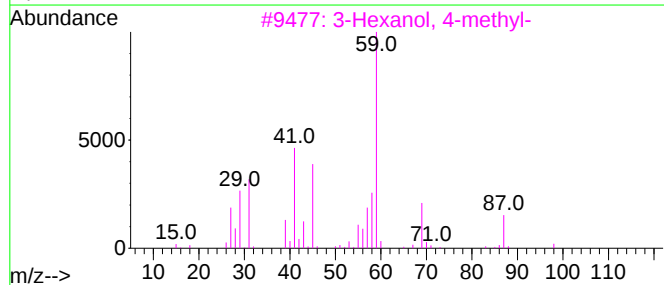
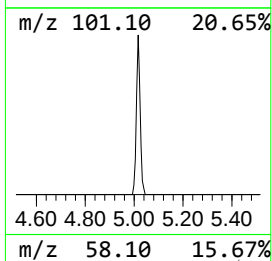
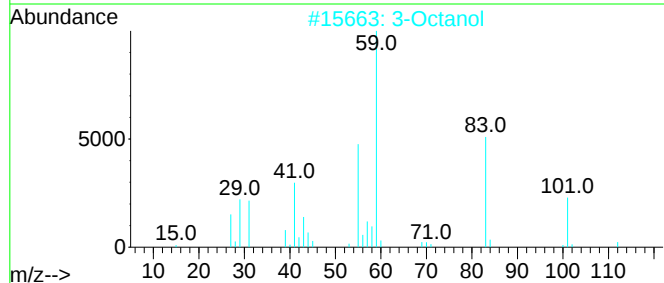
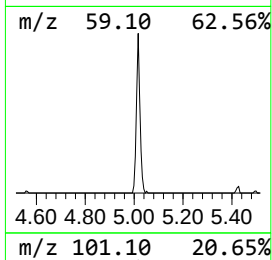
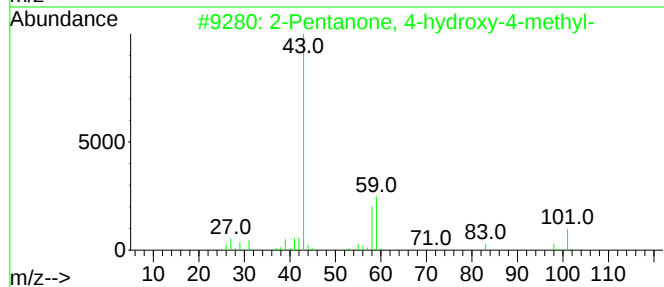
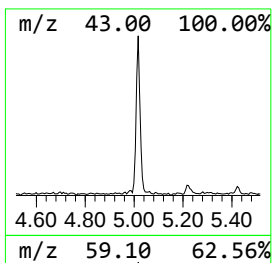
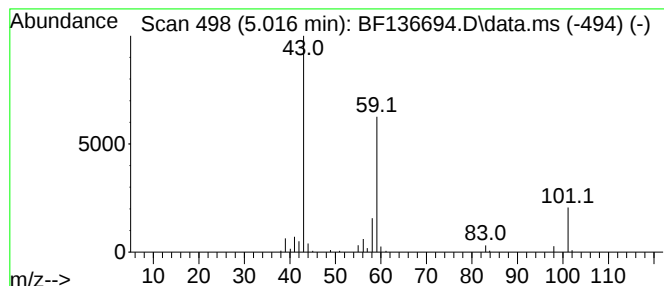
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.016	3.44 ng	65166	1,4-Dichlorobenzene-d4	6.787

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56		
2	3-Octanol	130	C8H18O	000589-98-0	33		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25		
4	5-Hexen-2-one	98	C6H10O	000109-49-9	9		
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9		



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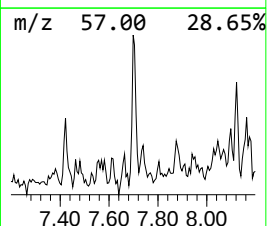
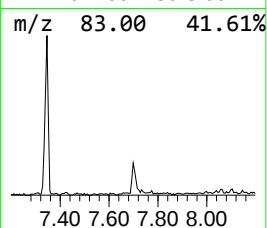
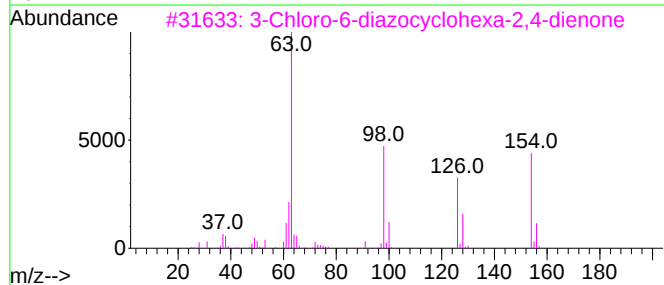
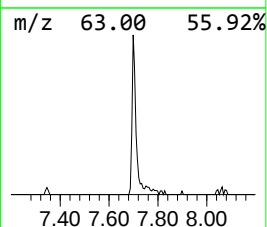
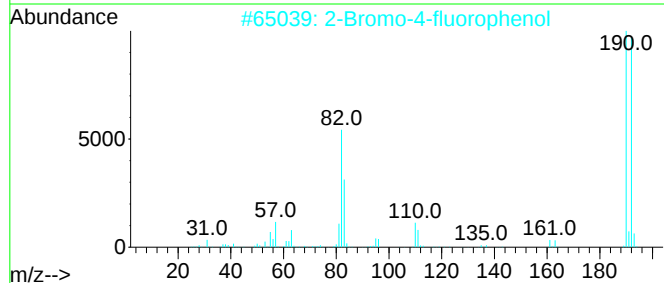
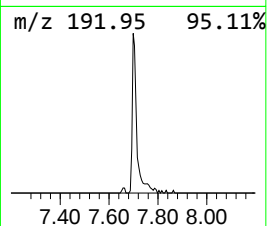
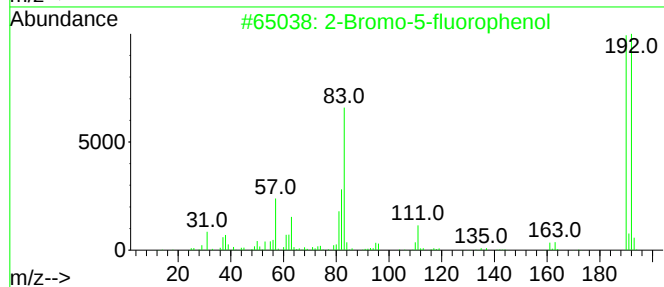
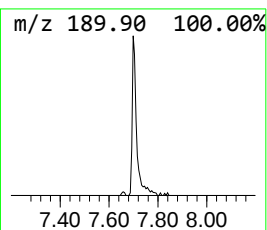
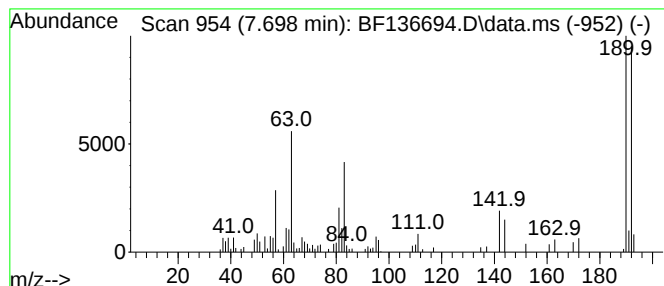
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Peak Number 2 2-Bromo-5-fluorophenol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.698	3.73 ng	82090	Naphthalene-d8	8.057

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Bromo-5-fluorophenol	190	C6H4BrFO	147460-41-1	53
2			2-Bromo-4-fluorophenol	190	C6H4BrFO	000496-69-5	46
3			3-Chloro-6-diazocyclohexa-2,4-di...	154	C6H3ClN2O	080090-95-5	25
4			3-Amino-5-bromo-2-fluoropyridine	190	C5H4BrFN2	884495-22-1	22
5			Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	17



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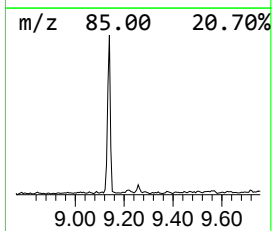
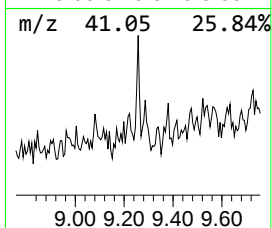
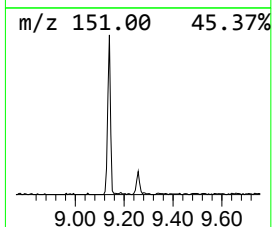
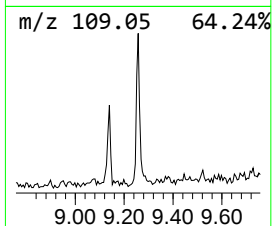
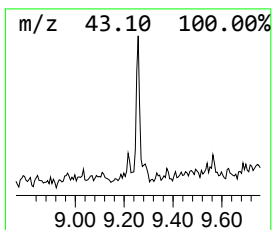
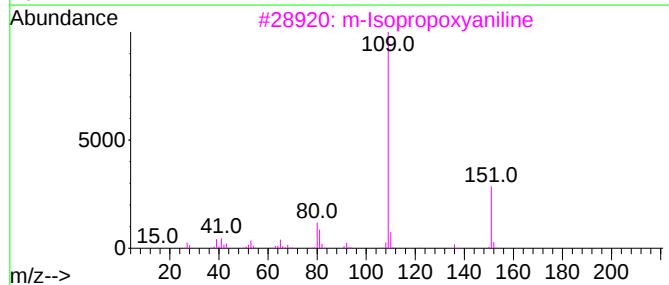
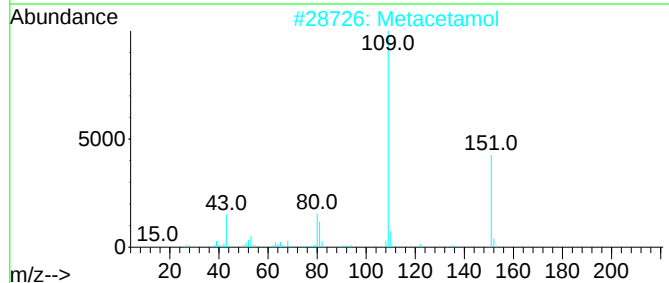
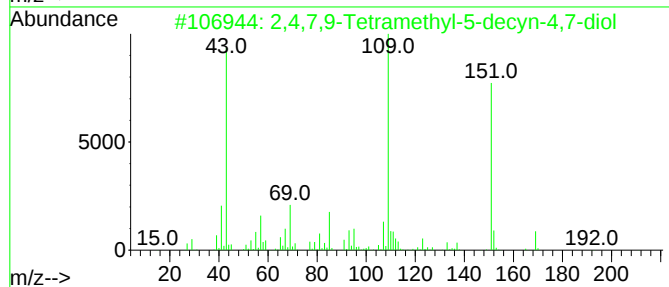
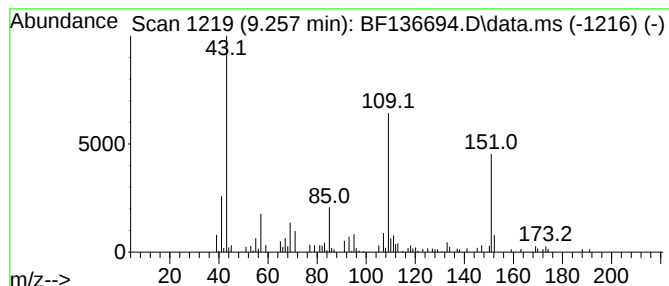
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.257	2.47 ng	48525	Acenaphthene-d10	9.816

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	64
2	Metacetamol	151	C8H9NO2		000621-42-1	50
3	m-Isopropoxyaniline	151	C9H13NO		041406-00-2	50
4	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3		1000107-08-7	40
5	Pyridine, 3-butyl-, 1-oxide	151	C9H13NO		031396-33-5	40



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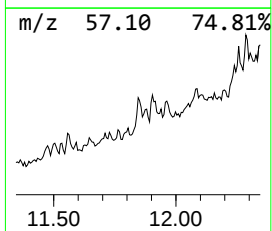
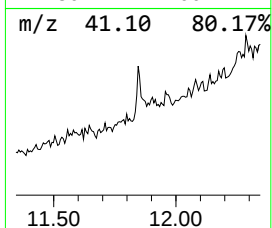
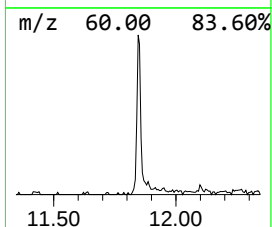
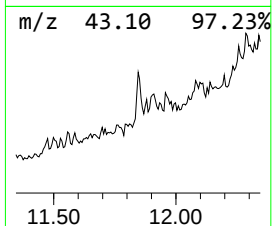
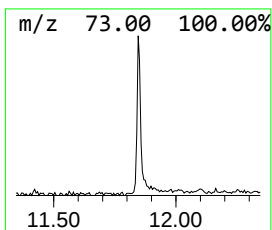
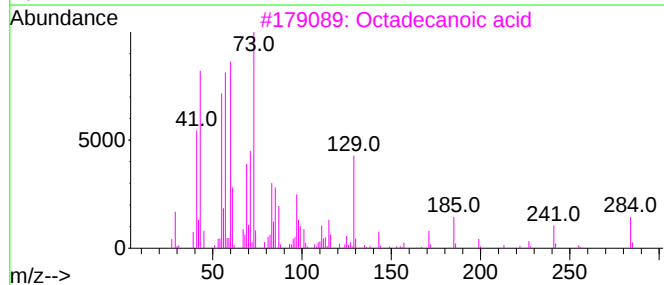
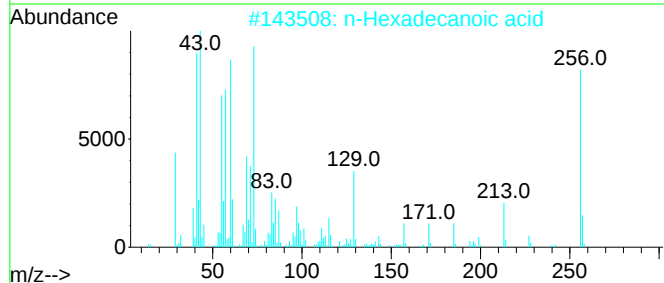
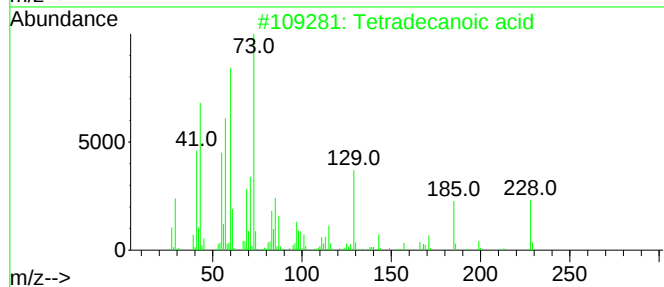
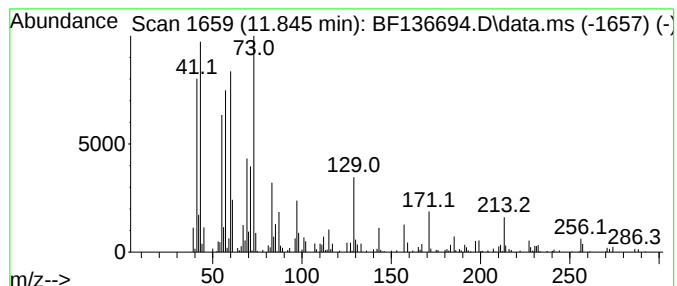
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Peak Number 4 Tetradecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.845	7.03 ng	125556	Phenanthrene-d10	11.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	87
3			Octadecanoic acid	284	C18H36O2	000057-11-4	64
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Decanoic acid, silver(1+) salt	278	C10H19AgO2	013126-67-5	53



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.016	3.4	ng	65166	1	6.787	379085	20.0
2-Bromo-5-fluor...	7.698	3.7	ng	82090	2	8.057	440631	20.0
2,4,7,9-Tetrame...	9.257	2.5	ng	48525	3	9.816	392971	20.0
Tetradecanoic acid	11.845	7.0	ng	125556	4	11.310	357000	20.0