

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100522\
 Data File : BF130542.D
 Acq On : 05 Oct 2022 21:46
 Operator : CG\JU
 Sample : N4977-01
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 251032-3

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-BF091422.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130542.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.798	458	461	474	rBV	127252	149622	5.99%	1.193%
2	5.234	532	535	547	rBV	766446	761128	30.48%	6.070%
3	6.275	709	712	723	rBV	426242	428256	17.15%	3.415%
4	6.634	769	773	776	rBV	472228	413493	16.56%	3.297%
5	7.198	865	869	872	rBV	1351877	1378445	55.20%	10.992%
6	7.845	974	979	987	rBV2	63580	213206	8.54%	1.700%
7	7.916	987	991	994	rVB	567925	503718	20.17%	4.017%
8	8.992	1170	1174	1177	rBV	3059016	2325782	93.13%	18.547%
9	9.116	1191	1195	1208	rVB	59019	74363	2.98%	0.593%
10	9.663	1281	1288	1299	rBV	617901	495678	19.85%	3.953%
11	10.451	1418	1422	1436	rBV	1429998	1233921	49.41%	9.840%
12	11.145	1536	1540	1548	rBV	532851	467224	18.71%	3.726%
13	11.545	1605	1608	1611	rBV	45195	38232	1.53%	0.305%
14	11.686	1628	1632	1634	rBV	184628	162739	6.52%	1.298%
15	11.716	1634	1637	1640	rVB	307774	260124	10.42%	2.074%
16	12.251	1723	1728	1731	rBV	86484	70640	2.83%	0.563%
17	12.339	1739	1743	1749	rVB2	41141	37206	1.49%	0.297%
18	12.469	1760	1765	1778	rBV	75278	97605	3.91%	0.778%
19	12.733	1805	1810	1813	rBV	2888493	2497234	100.00%	19.914%
20	13.774	1983	1987	1991	rBV	588272	523796	20.98%	4.177%
21	15.162	2219	2223	2233	rVB	325651	407710	16.33%	3.251%

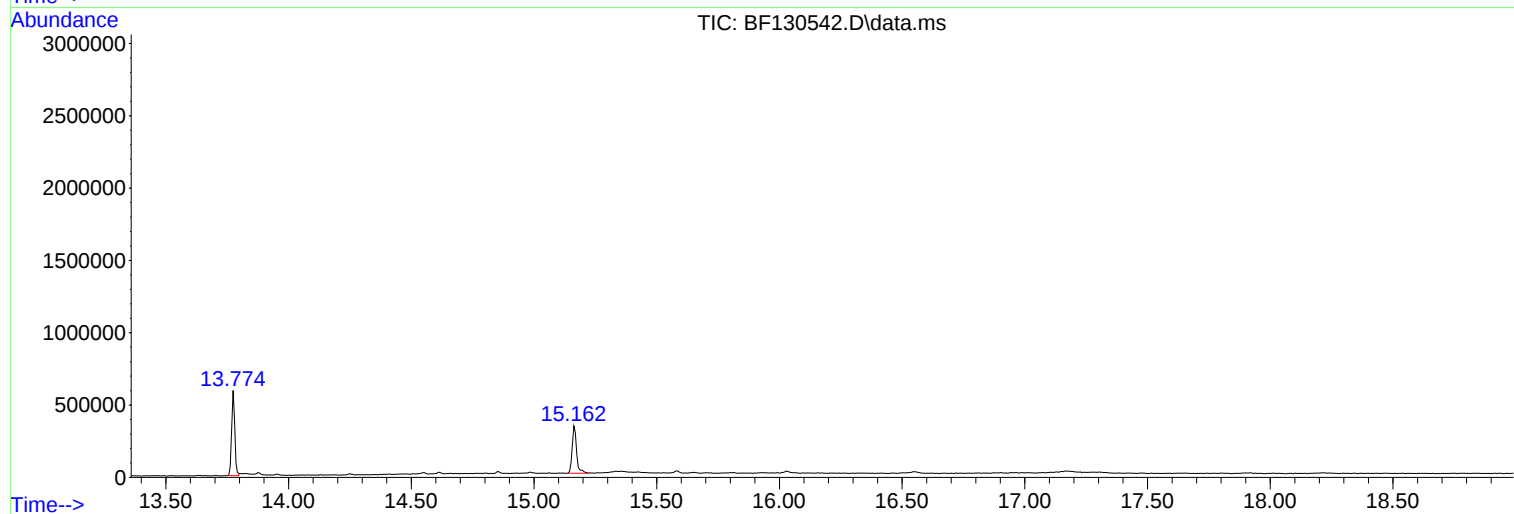
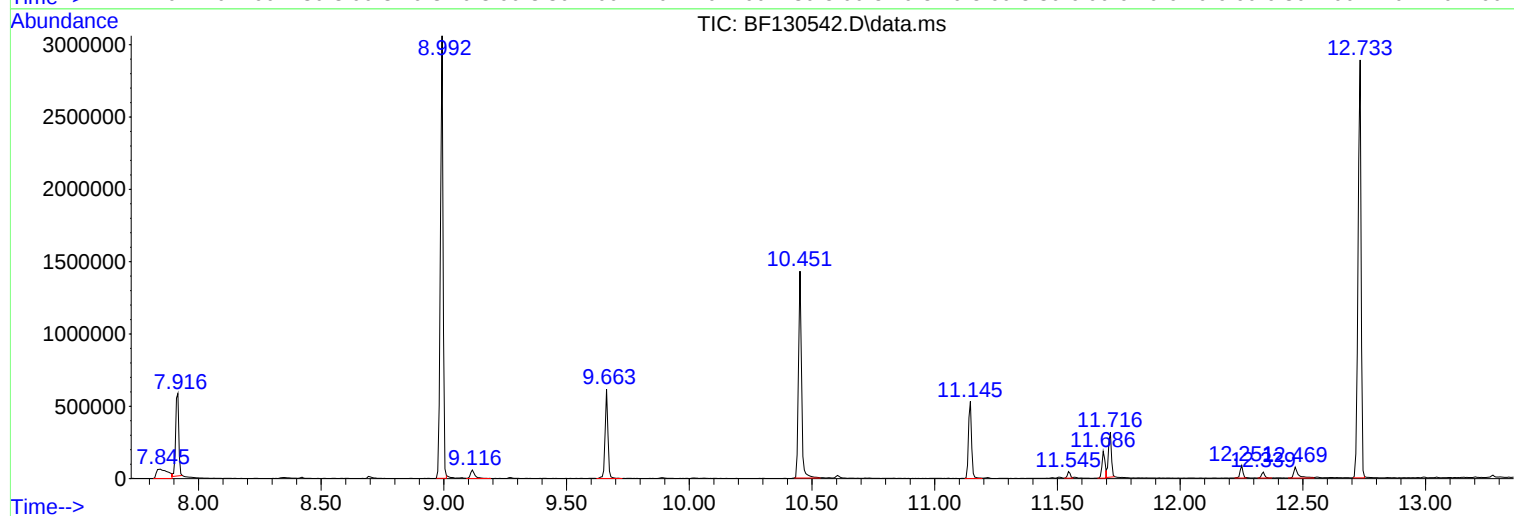
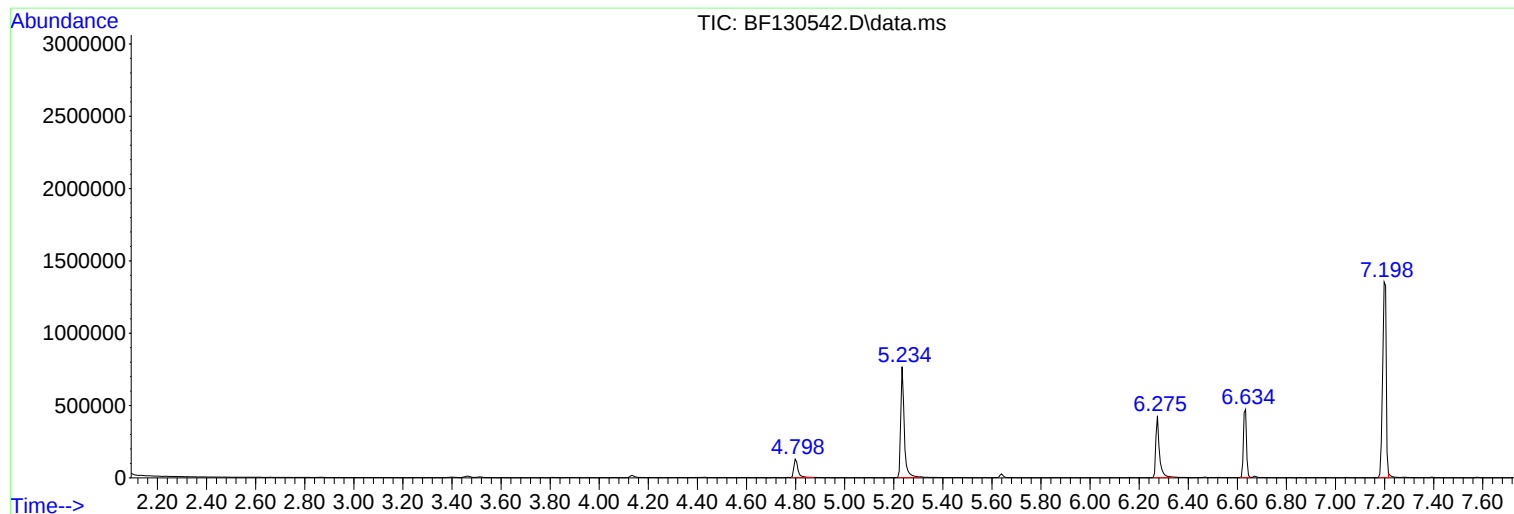
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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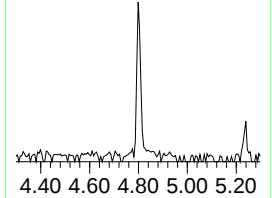
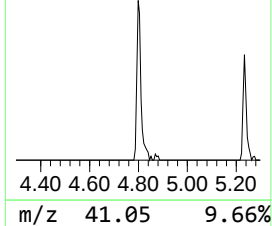
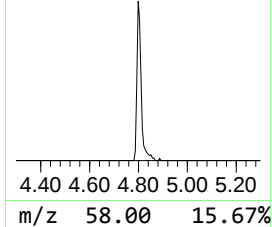
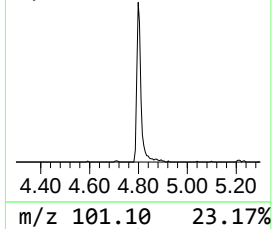
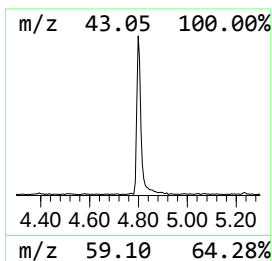
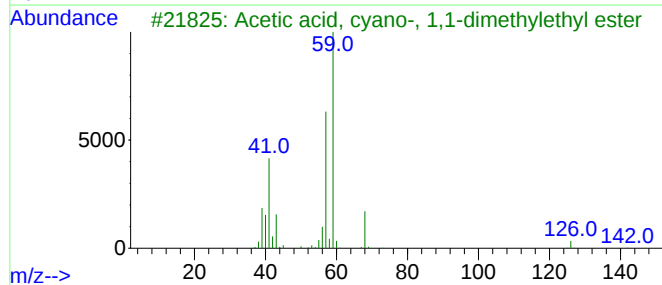
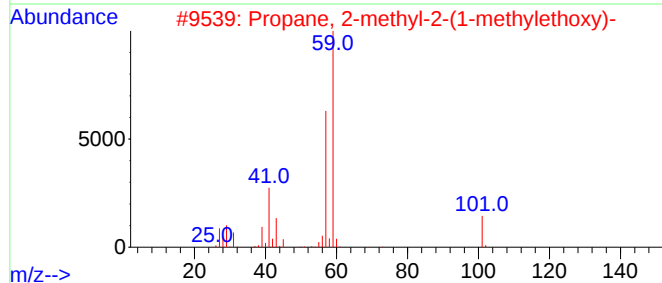
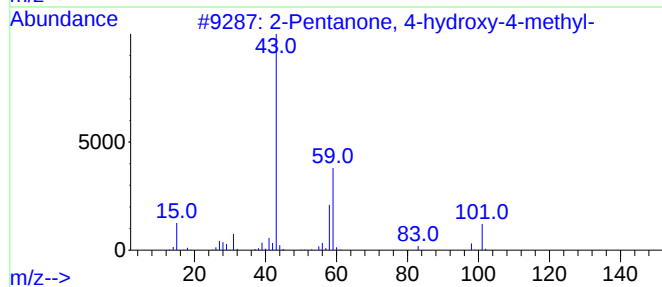
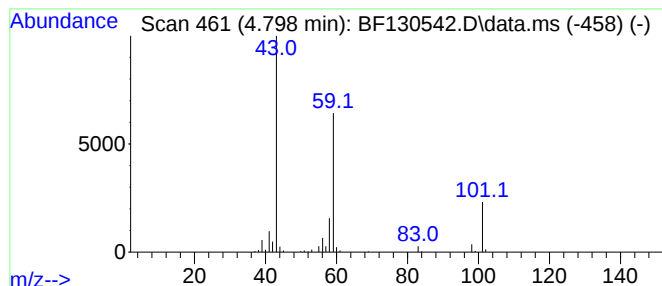
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.798	7.24 ng	149622	1,4-Dichlorobenzene-d4			6.634

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	40
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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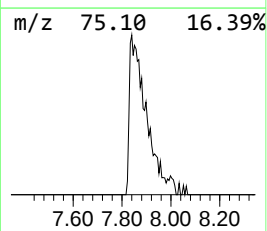
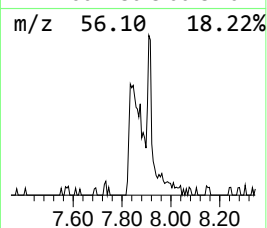
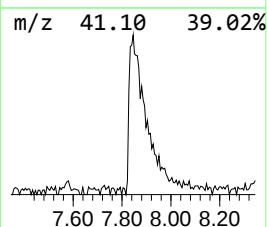
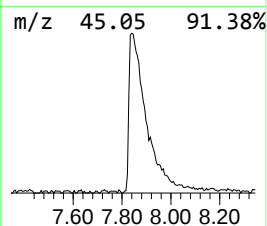
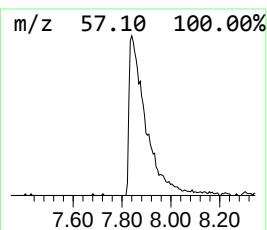
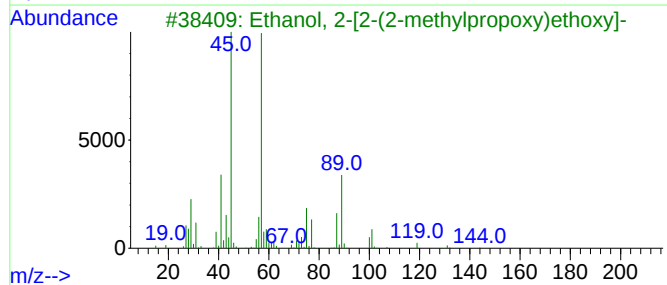
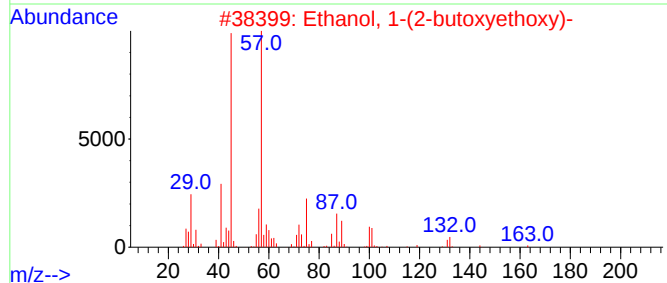
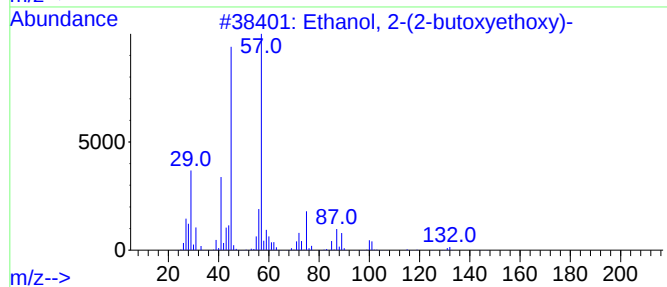
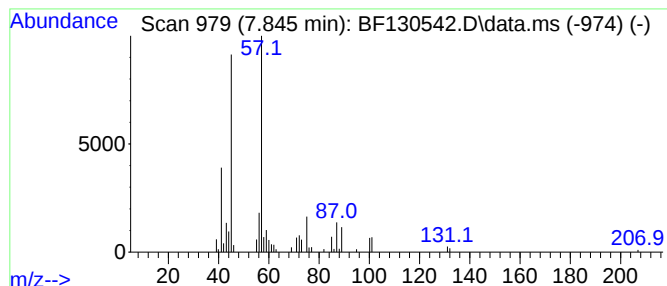
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Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.845	8.47 ng	213206	Naphthalene-d8	7.916

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	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	78
4			3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	59
5			2-Propanol, 1-(2-methylpropoxy)-	132	C7H16O2	023436-19-3	53



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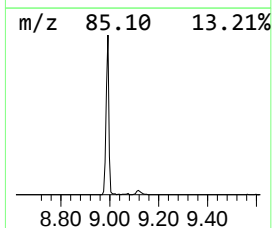
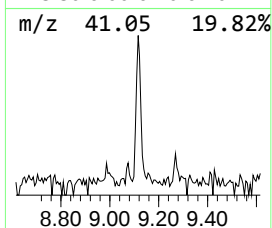
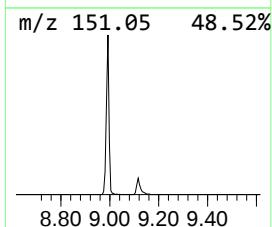
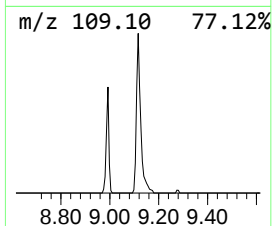
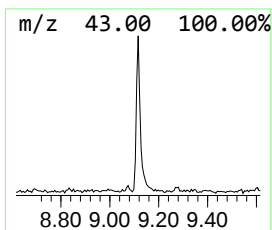
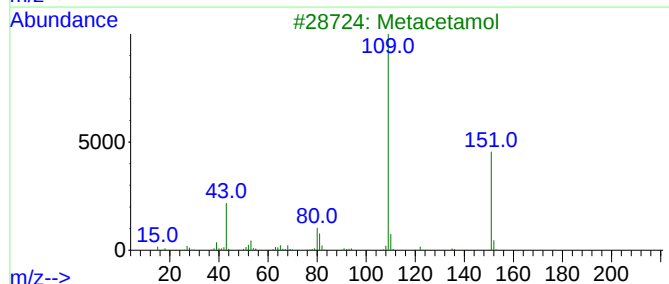
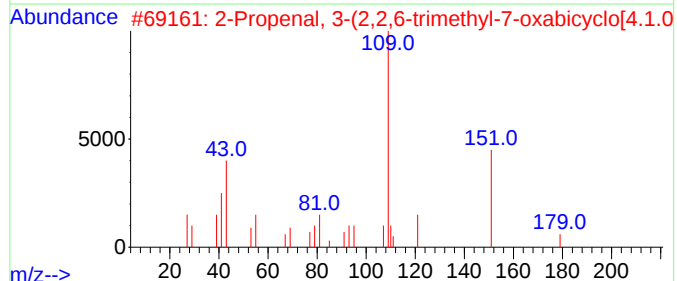
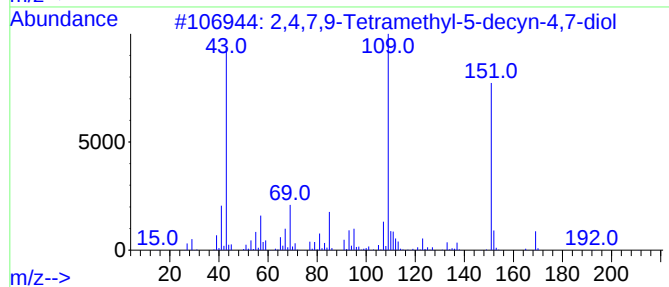
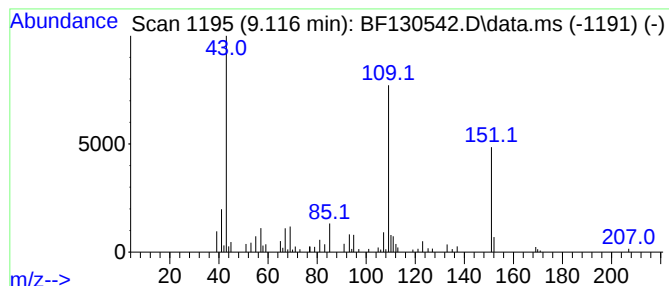
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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.
9.116	3.00 ng	74363	Acenaphthene-d10		9.663

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	2-Propenal, 3-(2,2,6-trimethyl-7...	194	C12H18O2	055759-91-6	64	
3	Metacetamol	151	C8H9NO2	000621-42-1	59	
4	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2	001006-96-8	59	
5	Butanamide, N-acetyl-N-(4-hydrox...	221	C12H15NO3	1000107-08-7	59	



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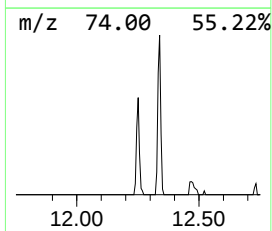
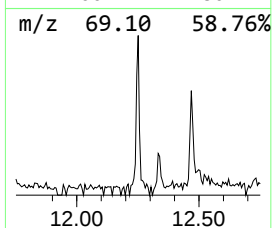
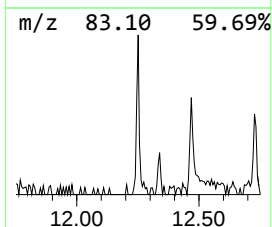
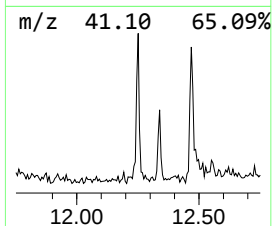
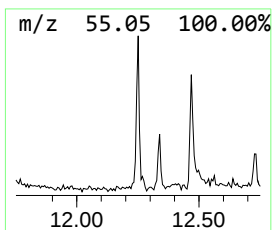
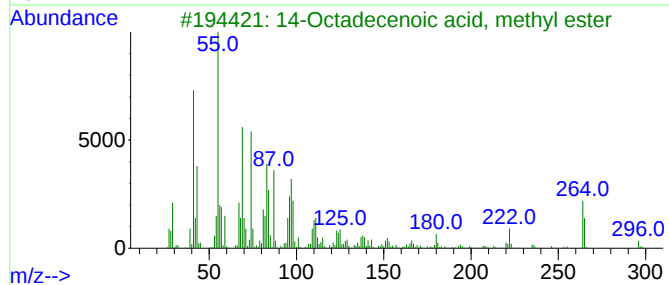
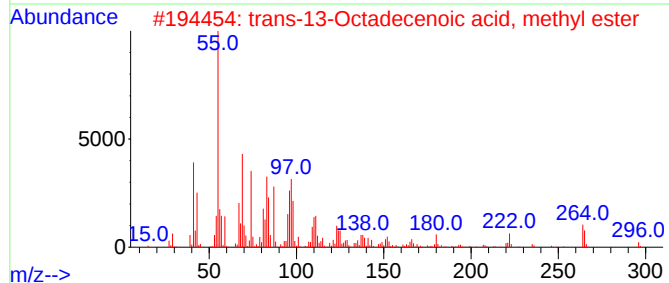
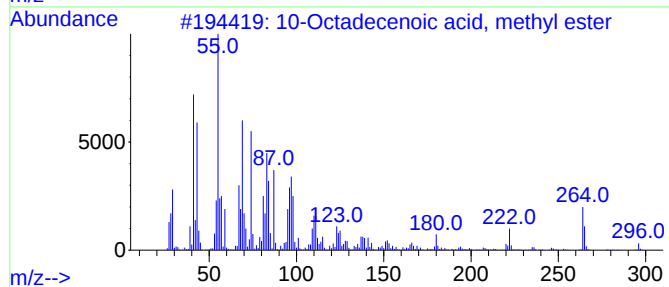
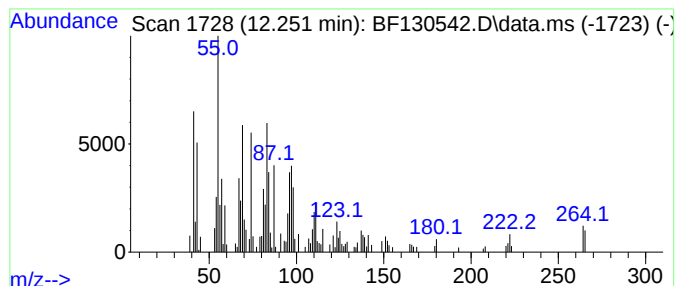
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Peak Number 4 10-Octadecenoic acid, methyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.251	3.02 ng	70640	Phenanthrene-d10	11.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	91
2			trans-13-Octadecenoic acid, methyl ester	296	C19H36O2	1000333-61-3	91
3			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	91
4			9-Octadecenoic acid (Z)-, methyl ester	296	C19H36O2	000112-62-9	87
5			9-Hexadecenoic acid, methyl ester	268	C17H32O2	001120-25-8	83



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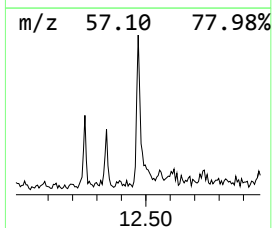
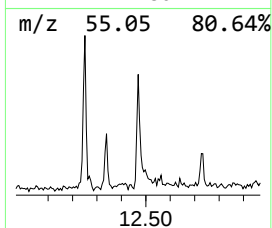
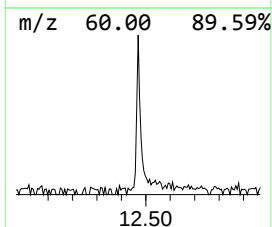
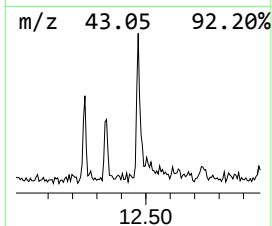
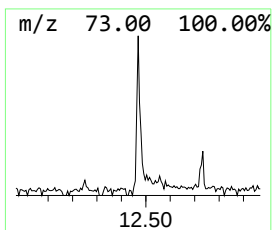
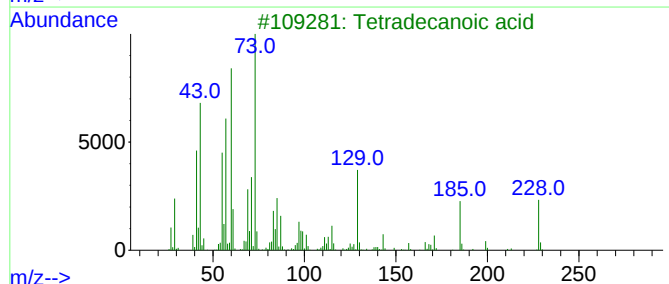
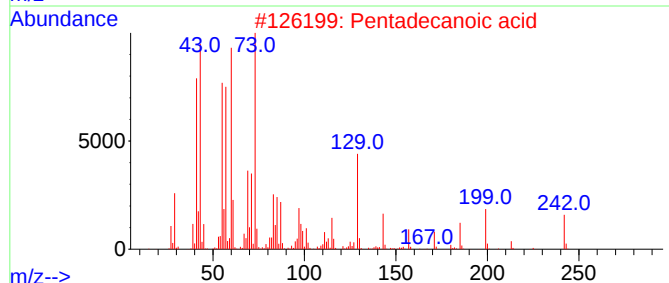
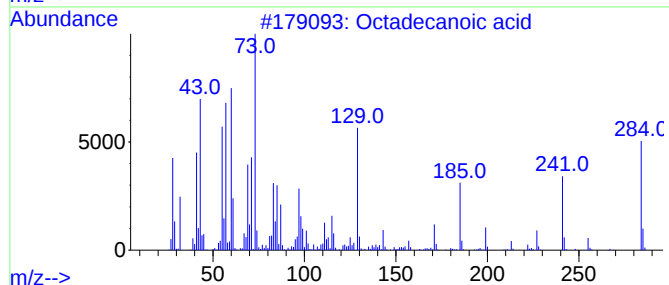
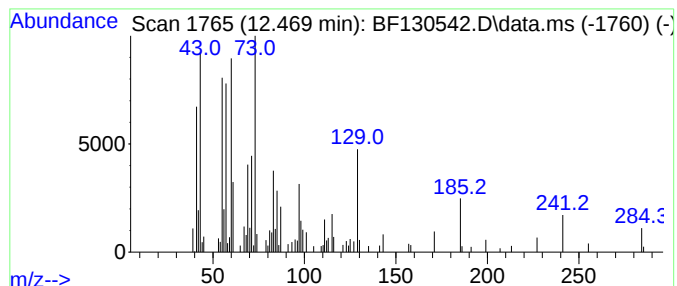
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Peak Number 5 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.469	3.73 ng	97605	Chrysene-d12	13.774

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.798	7.2	ng	149622	1	6.634	413493	20.0
Ethanol, 2-(2-b...	7.845	8.5	ng	213206	2	7.916	503718	20.0
2,4,7,9-Tetrame...	9.116	3.0	ng	74363	3	9.663	495678	20.0
10-Octadecenoic...	12.251	3.0	ng	70640	4	11.145	467224	20.0
Octadecanoic acid	12.469	3.7	ng	97605	5	13.774	523796	20.0