

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110921\
 Data File : BP007888.D
 Acq On : 09 Nov 2021 13:07
 Operator : CG/JU
 Sample : M4477-04
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 T1-B1-S

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_P\Methods\8270E-BP110221.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP007888.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.446	361	367	382	rVB	1266067	1868970	49.92%	8.354%
2	7.040	629	638	648	rBV	1112926	1802136	48.14%	8.056%
3	7.863	771	778	787	rBV	477524	749994	20.03%	3.353%
4	9.016	966	974	984	rBV	650108	1079957	28.85%	4.828%
5	10.445	1211	1217	1226	rBV	258875	409171	10.93%	1.829%
6	10.663	1246	1254	1267	rVB	528657	908684	24.27%	4.062%
7	13.122	1665	1672	1683	rBV	1646133	2432268	64.97%	10.872%
8	13.404	1714	1720	1726	rBV2	34317	56741	1.52%	0.254%
9	14.339	1861	1879	1886	rBV5	29736	121643	3.25%	0.544%
10	14.498	1899	1906	1917	rVB	779120	1121150	29.95%	5.012%
11	15.992	2154	2160	2180	rVB	1200183	1836210	49.05%	8.208%
12	17.251	2368	2374	2388	rBV	895273	1321468	35.30%	5.907%
13	17.374	2388	2395	2402	rVB7	25509	45932	1.23%	0.205%
14	17.933	2486	2490	2494	rVB	62825	71851	1.92%	0.321%
15	18.145	2522	2526	2533	rBV	85822	139777	3.73%	0.625%
16	18.216	2535	2538	2543	rVB	29347	40959	1.09%	0.183%
17	19.063	2679	2682	2686	rVB	143087	159333	4.26%	0.712%
18	19.198	2701	2705	2709	rBV	35462	43587	1.16%	0.195%
19	19.386	2733	2737	2742	rBV3	39330	61075	1.63%	0.273%
20	19.816	2805	2810	2818	rBV	3089419	3743885	100.00%	16.735%
21	20.568	2934	2938	2945	rVB	215754	240767	6.43%	1.076%
22	21.057	3018	3021	3027	rBV3	122743	162992	4.35%	0.729%
23	21.345	3065	3070	3081	rBV	1396449	1822437	48.68%	8.146%
24	23.762	3474	3481	3491	rVB2	1037134	2129933	56.89%	9.521%

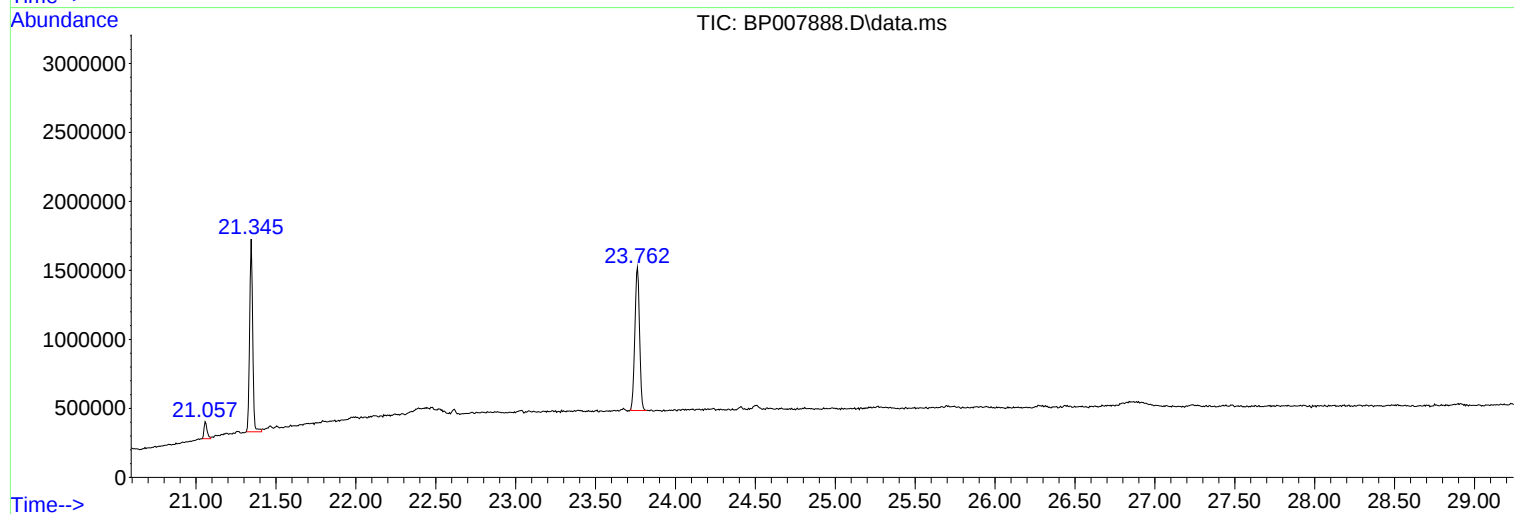
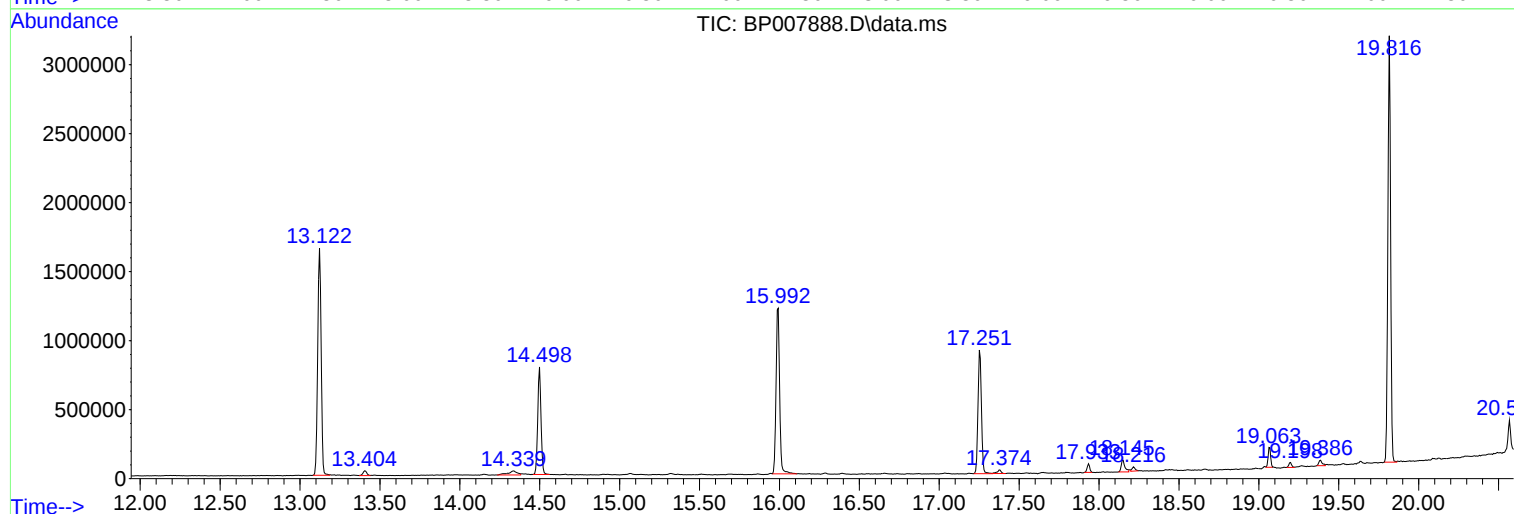
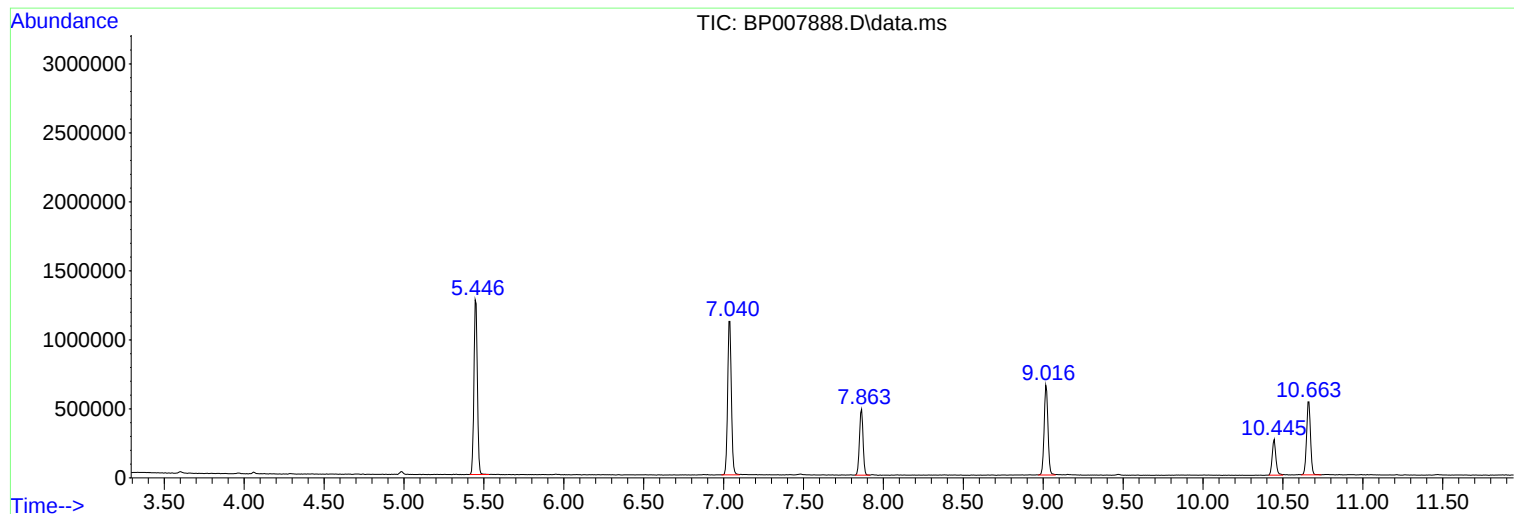
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP110221.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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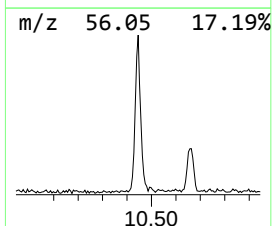
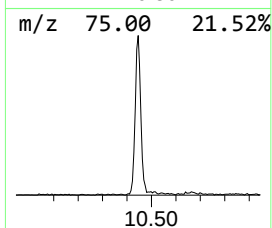
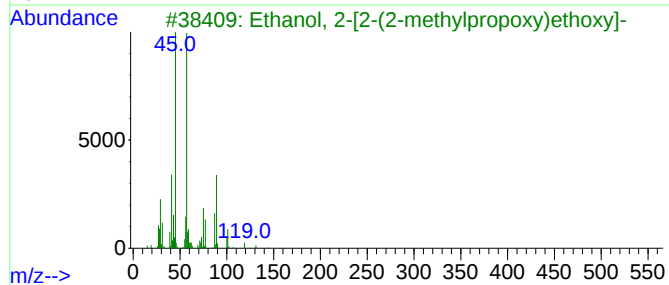
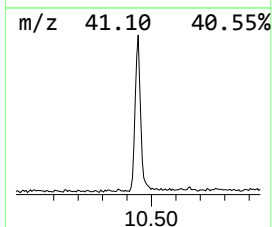
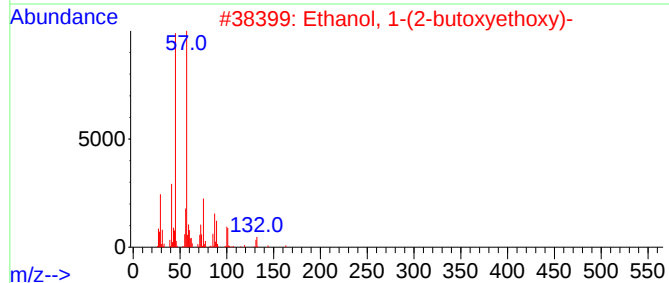
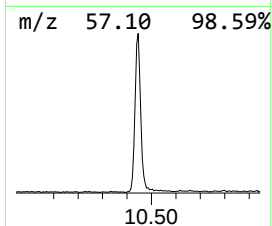
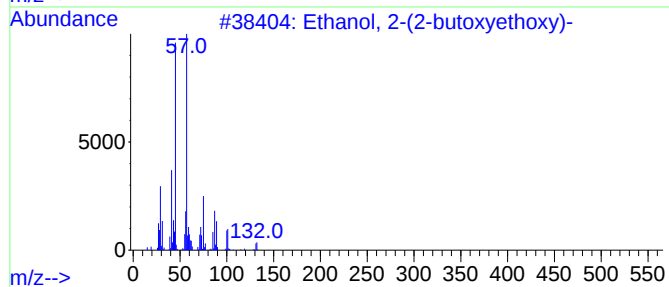
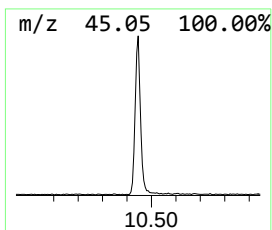
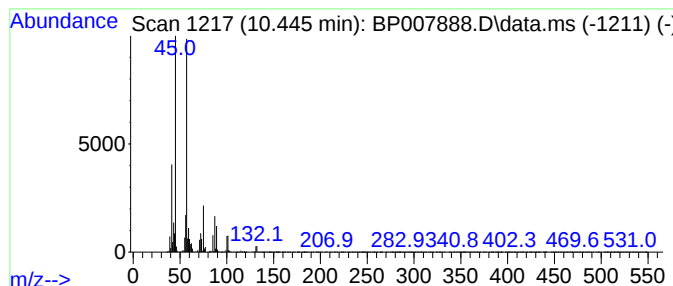
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.445	9.01 ng	409171	Naphthalene-d8	10.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	91
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	90
3			Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	72
4			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
5			Propanoic acid, 2-hydroxy-, 2-me...	146	C7H14O3	000585-24-0	53



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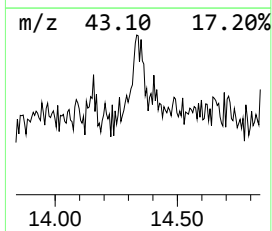
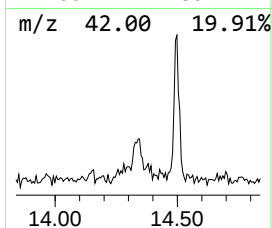
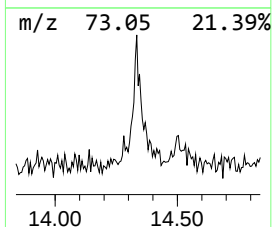
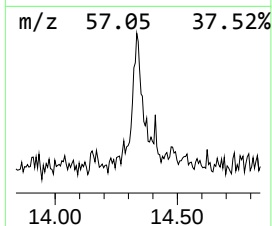
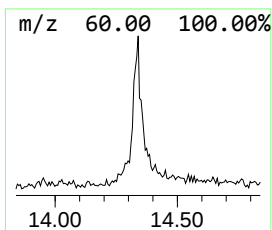
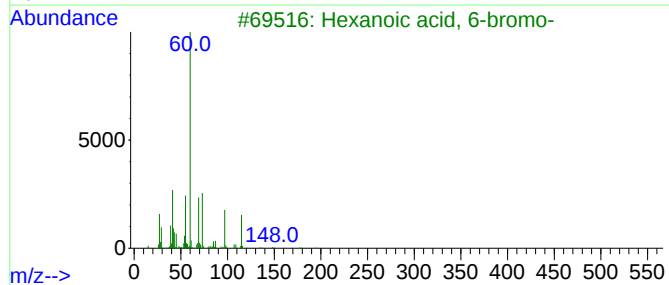
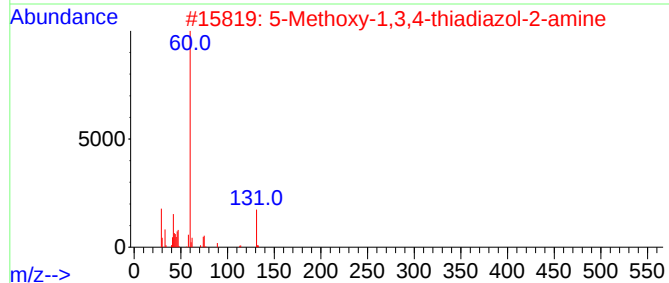
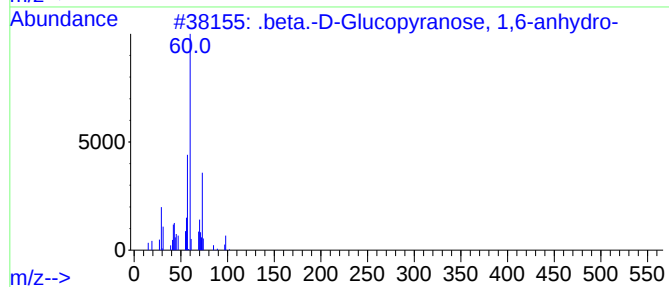
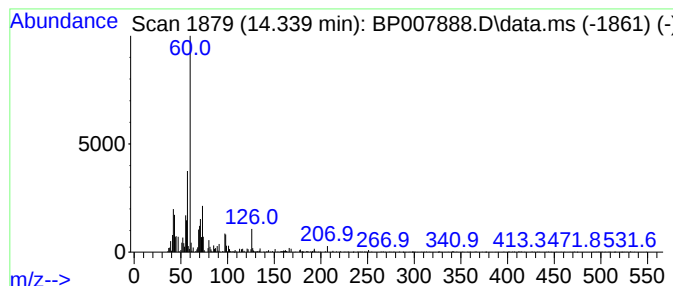
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Peak Number 2 .beta.-D-Glucopyranose, 1,6... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.339	2.17 ng	121643	Acenaphthene-d10	14.498

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-D-Glucopyranose, 1,6-anhy...	162	C6H10O5	000498-07-7	59
2		5-Methoxy-1,3,4-thiadiazol-2-amine	131	C3H5N3OS	016841-84-2	50
3		Hexanoic acid, 6-bromo-	194	C6H11BrO2	004224-70-8	42
4		(S)-3-Aminotetrahydrofuran, Ac d...	129	C6H11NO2	1000496-60-7	40
5		Methyl-.beta.-D-thiogalactoside	194	C7H14O6	001824-94-8	40



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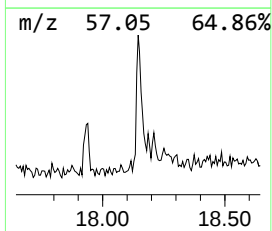
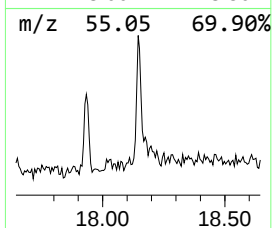
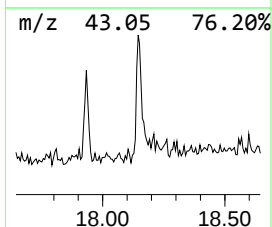
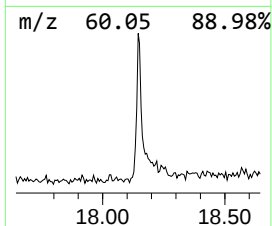
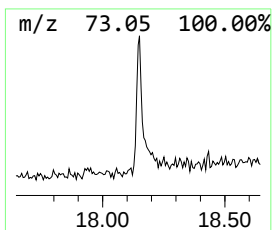
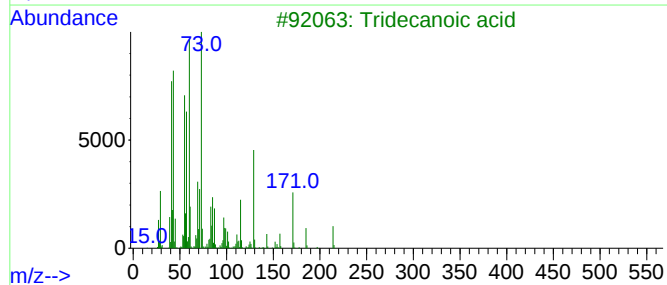
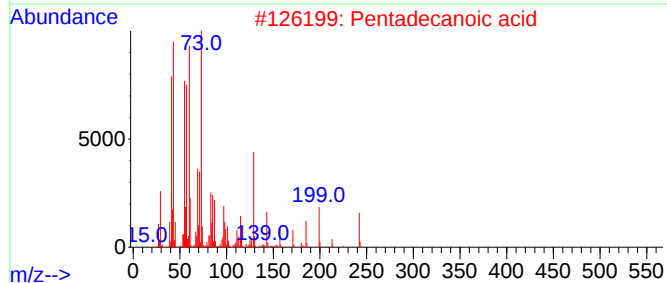
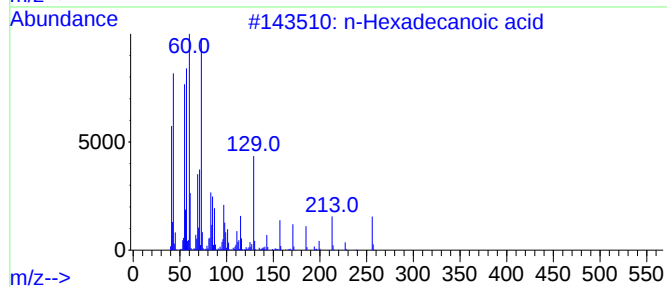
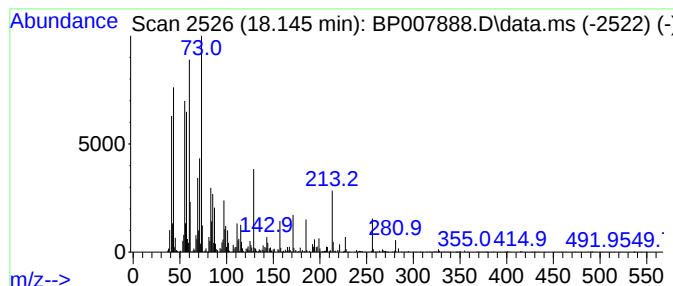
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	2.12 ng	139777	Phenanthrene-d10	17.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Octadecanoic acid	284	C18H36O2	000057-11-4	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	81



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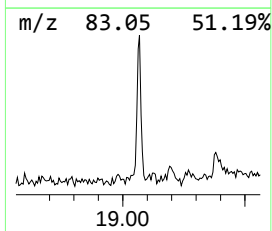
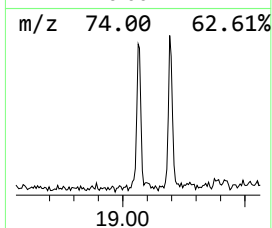
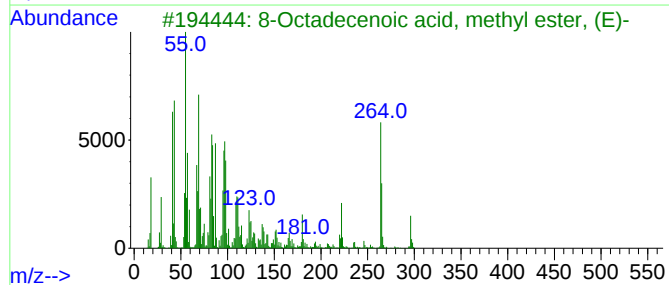
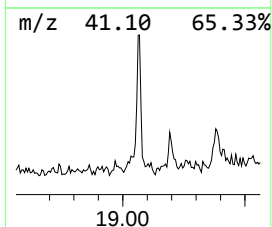
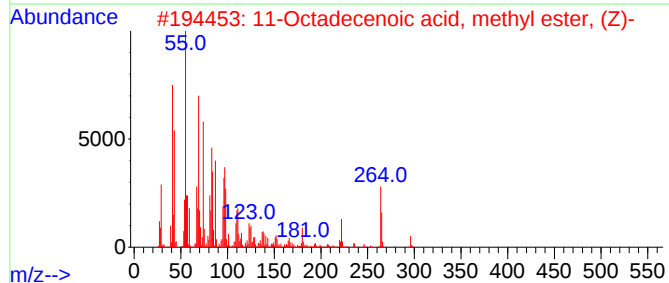
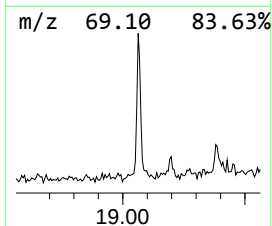
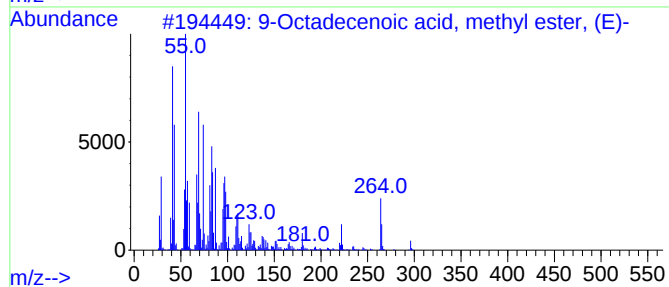
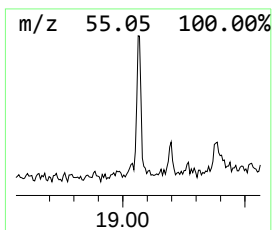
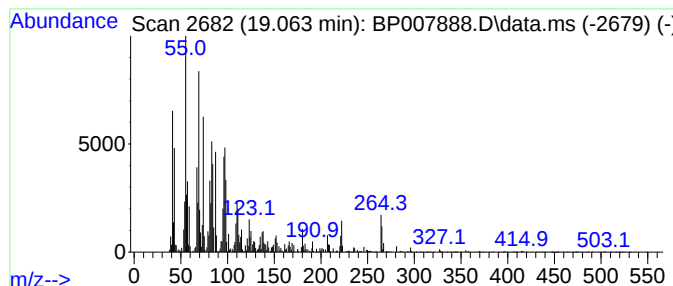
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Peak Number 4 9-Octadecenoic acid, methyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.063	2.41 ng	159333	Phenanthrene-d10	17.251

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
2			11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
3			8-Octadecenoic acid, methyl este...	296	C19H36O2	026528-50-7	99
4			cis-12-Octadecenoic acid methyl ...	296	C19H36O2	1000427-68-4	99
5			10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99



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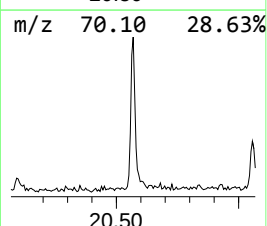
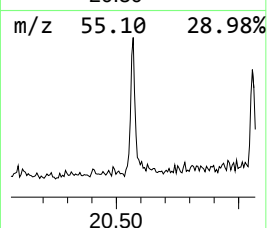
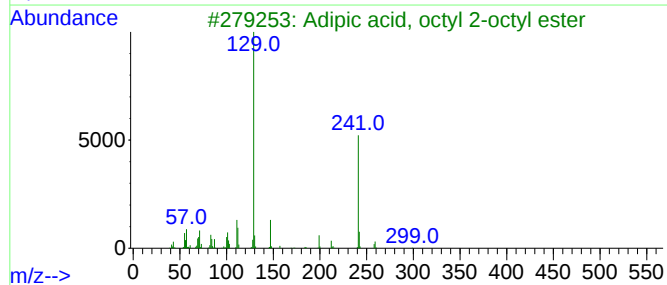
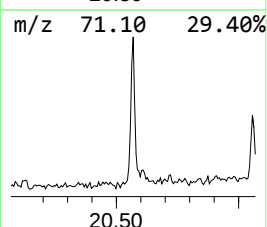
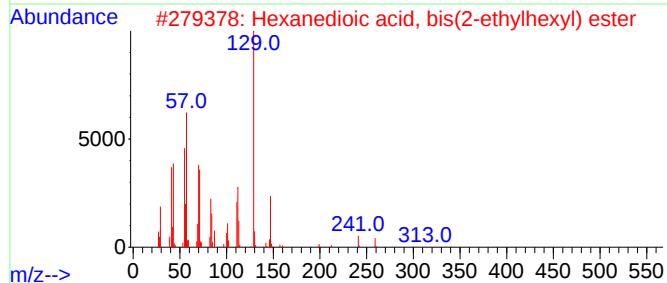
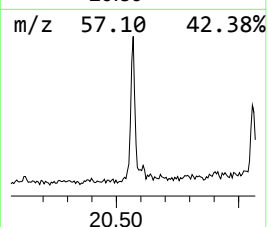
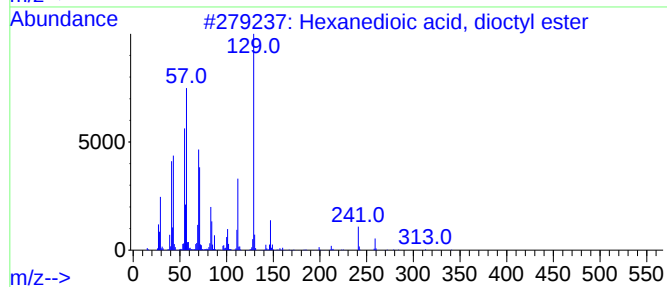
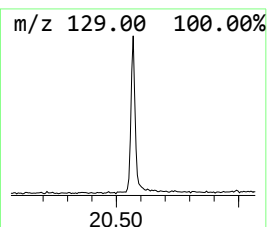
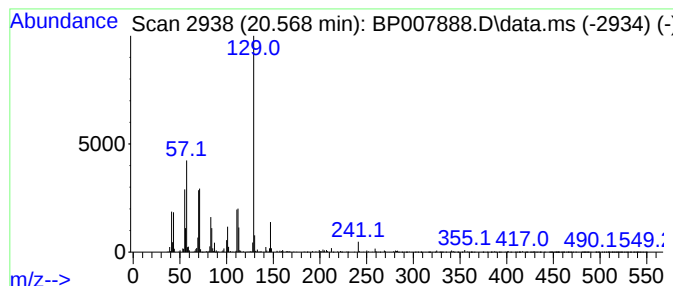
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Peak Number 5 Hexanedioic acid, dioctyl e... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.568	2.64 ng	240767	Chrysene-d12	21.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	91
2			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	89
3			Adipic acid, octyl 2-octyl ester	370	C22H42O4	1000324-45-0	64
4			Diisooctyl adipate	370	C22H42O4	001330-86-5	64
5			Adipic acid, 2-ethylhexyl isobut...	314	C18H34O4	1010324-48-0	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethanol, 2-(2-b...	10.445	9.0	ng	409171	2	10.663	908684	20.0
.beta.-D-Glucop...	14.339	2.2	ng	121643	3	14.498	1121150	20.0
n-Hexadecanoic ...	18.145	2.1	ng	139777	4	17.251	1321470	20.0
9-Octadecenoic ...	19.063	2.4	ng	159333	4	17.251	1321470	20.0
Hexanedioic aci...	20.568	2.6	ng	240767	5	21.345	1822440	20.0