

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042321\
 Data File : BP005395.D
 Acq On : 23 Apr 2021 15:58
 Operator : CG/JU
 Sample : M2150-02
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TWP-20

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-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005395.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	359	365	378	rBV	298711	431122	17.14%	4.497%
2	6.822	628	635	653	rBV3	163581	322687	12.83%	3.366%
3	7.634	766	773	781	rBV	109778	169054	6.72%	1.764%
4	8.799	963	971	983	rBV	444508	718909	28.58%	7.499%
5	10.422	1239	1247	1252	rBV	119309	198217	7.88%	2.068%
6	10.475	1252	1256	1262	rVB	31256	52002	2.07%	0.542%
7	12.099	1525	1532	1542	rBV3	37314	68755	2.73%	0.717%
8	12.316	1564	1569	1576	rVB2	17547	30918	1.23%	0.323%
9	12.916	1663	1671	1681	rBV	978338	1394036	55.41%	14.542%
10	13.763	1807	1815	1825	rBV	24865	39852	1.58%	0.416%
11	14.304	1899	1907	1913	rBV	164097	251888	10.01%	2.628%
12	14.363	1913	1917	1925	rVB	20390	32971	1.31%	0.344%
13	15.363	2081	2087	2093	rVB2	19054	28593	1.14%	0.298%
14	15.804	2156	2162	2182	rBV	977835	1419877	56.44%	14.812%
15	17.069	2370	2377	2382	rBV	241424	337588	13.42%	3.522%
16	17.110	2382	2384	2390	rVB	23265	29075	1.16%	0.303%
17	17.975	2525	2531	2539	rBV	121383	180548	7.18%	1.883%
18	19.216	2738	2742	2754	rBV	65361	96706	3.84%	1.009%
19	19.651	2810	2816	2827	rBV	2303915	2515862	100.00%	26.245%
20	20.886	3023	3026	3034	rVB2	74637	132368	5.26%	1.381%
21	20.957	3035	3038	3045	rVB	75846	92409	3.67%	0.964%
22	21.175	3070	3075	3083	rBV	420193	518427	20.61%	5.408%
23	23.433	3453	3459	3467	rVB	271977	524297	20.84%	5.469%

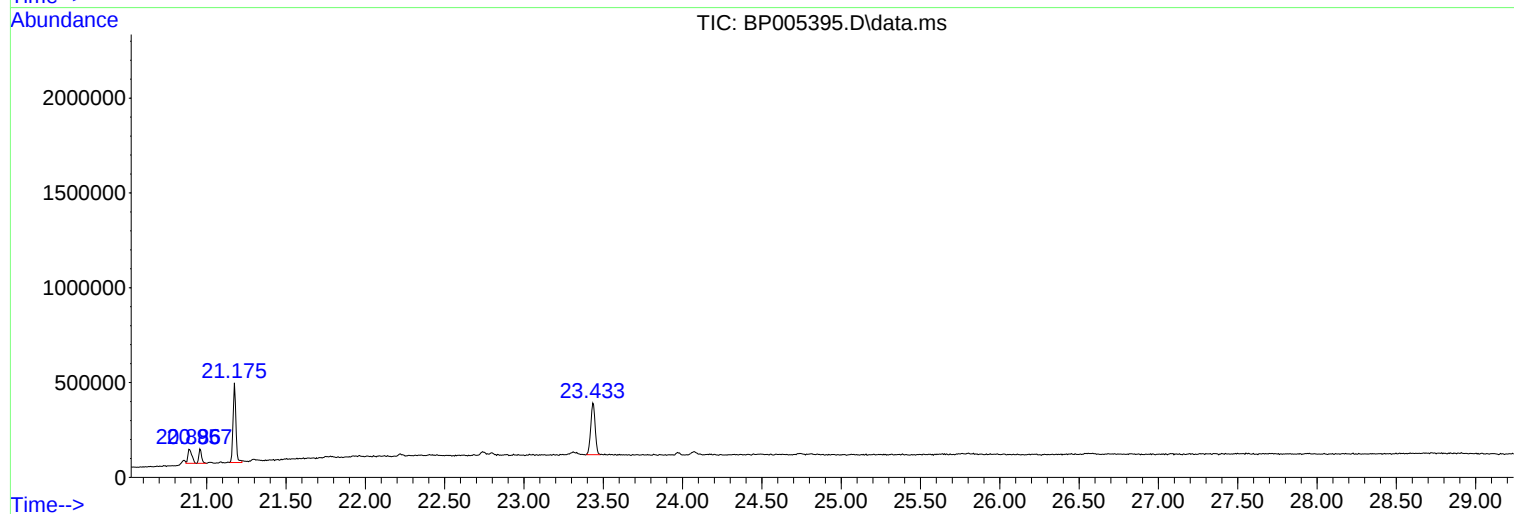
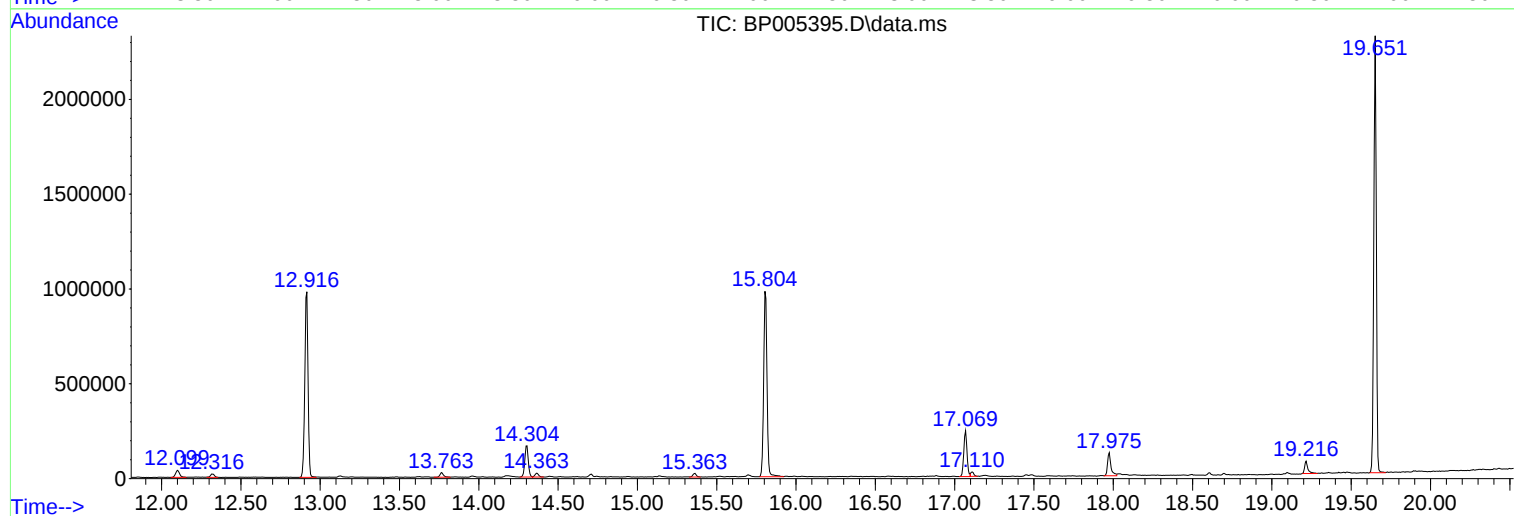
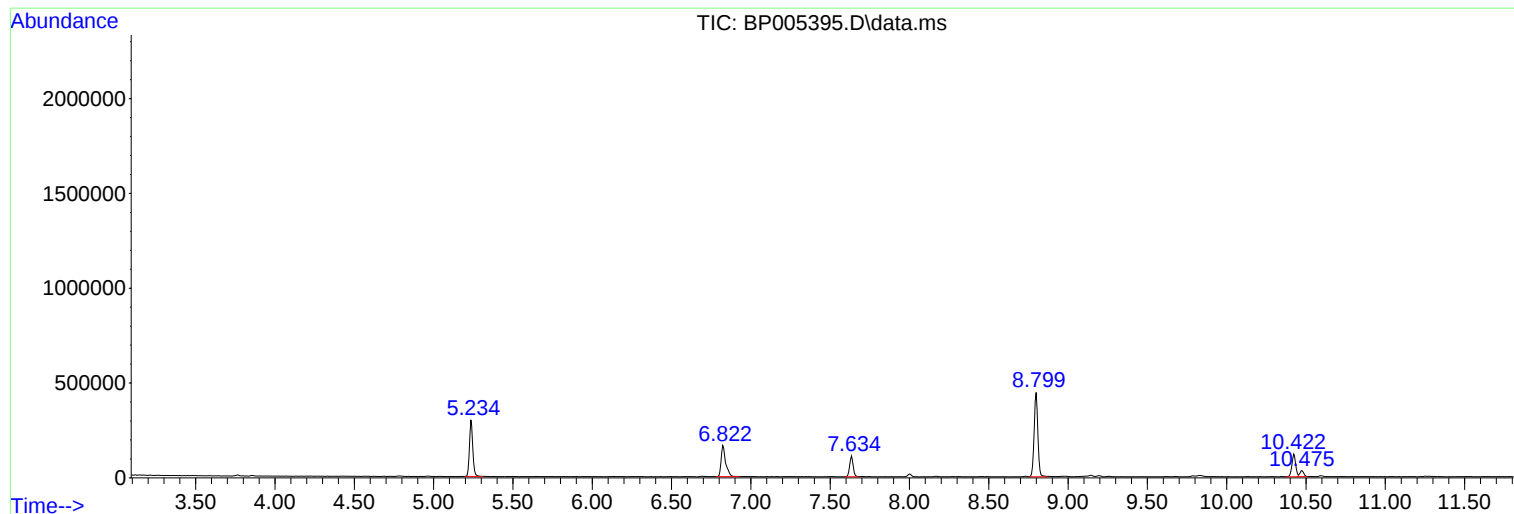
Sum of corrected areas: 9586161

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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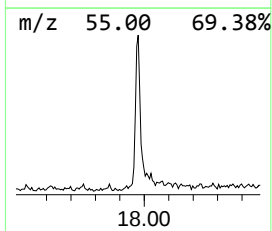
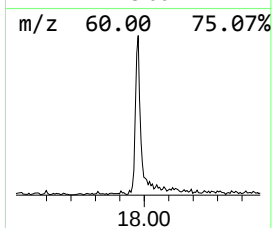
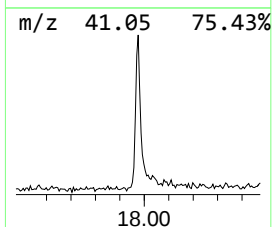
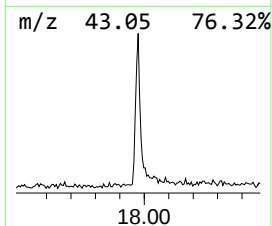
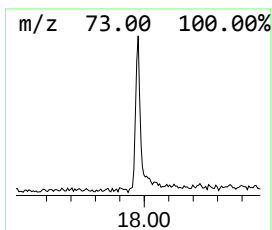
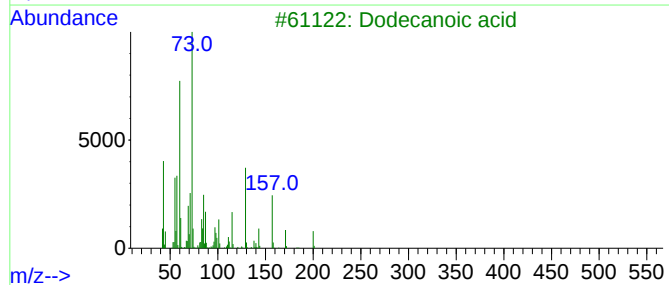
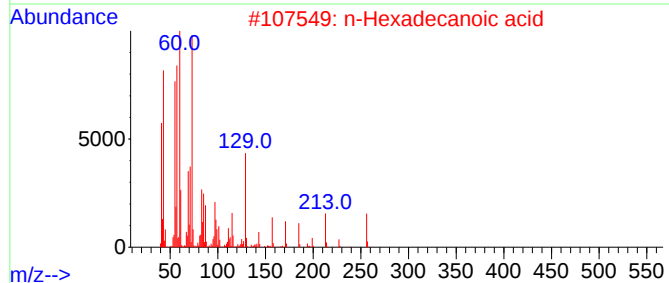
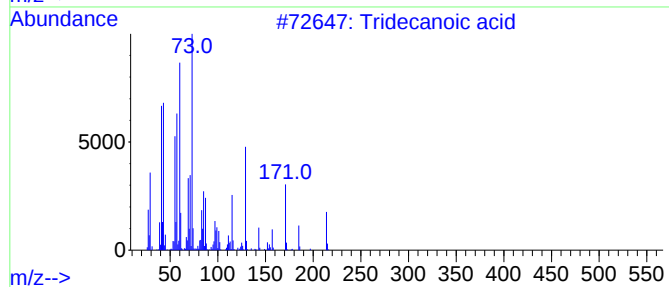
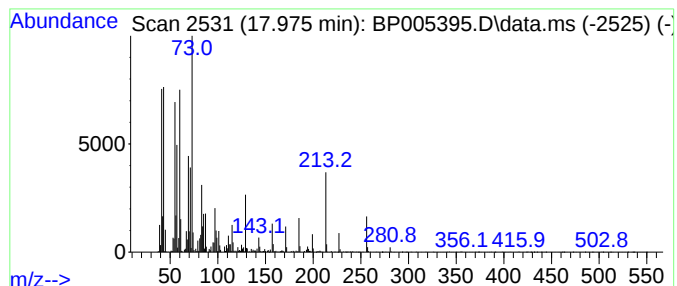
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Tridecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.975	10.70 ng	180548	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tridecanoic acid	214	C13H26O2	000638-53-9	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Dodecanoic acid	200	C12H24O2	000143-07-7	70
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	64
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	64



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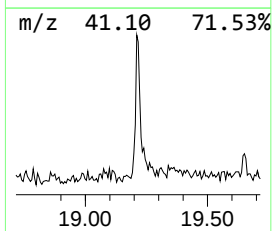
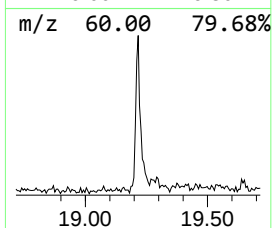
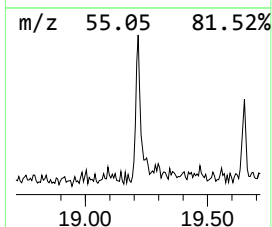
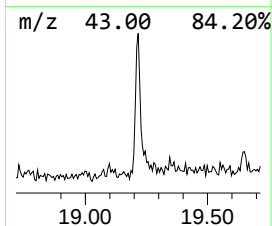
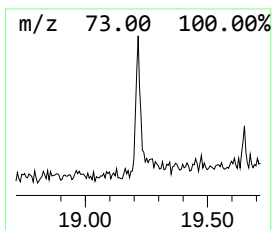
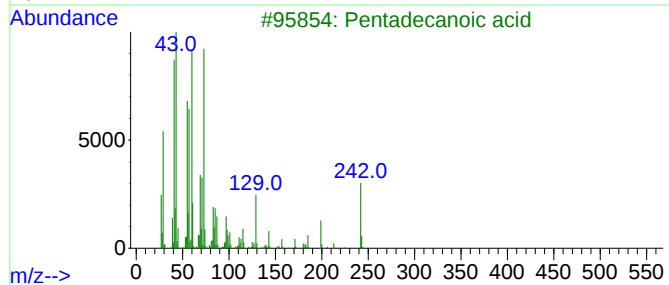
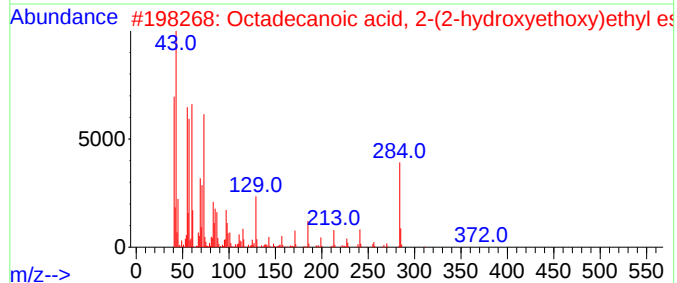
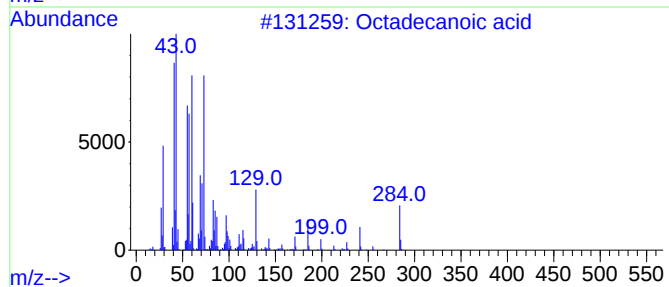
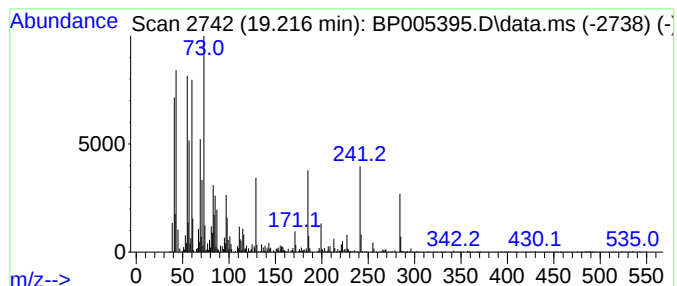
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Peak Number 3 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.216	3.73 ng	96706	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	90
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	64
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	60
4			Undecanoic acid	186	C11H22O2	000112-37-8	60
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



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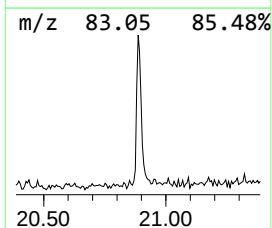
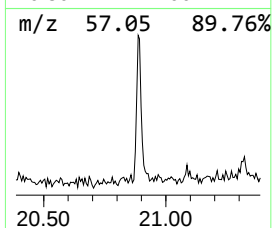
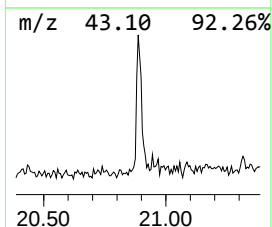
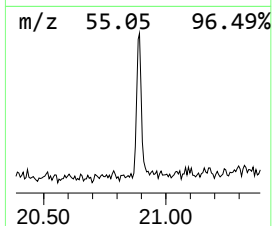
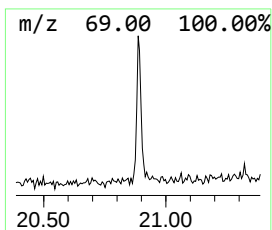
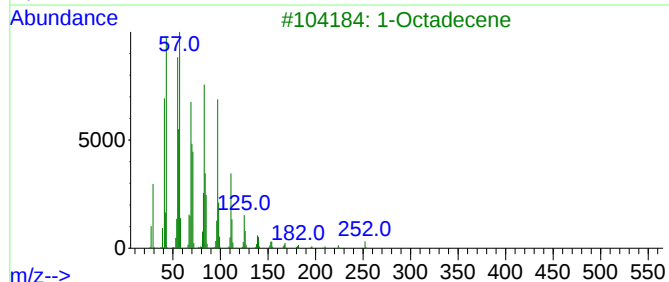
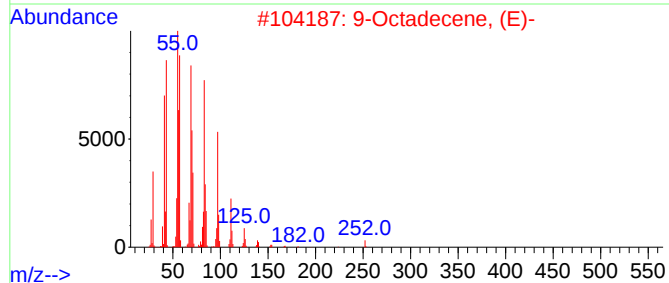
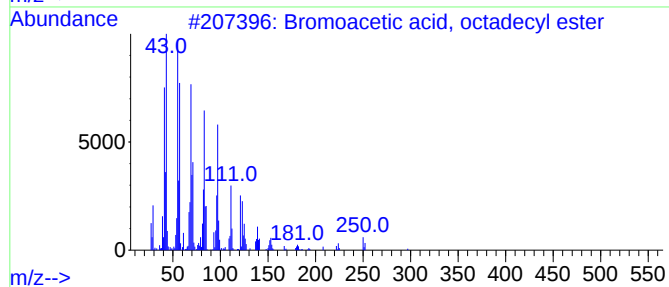
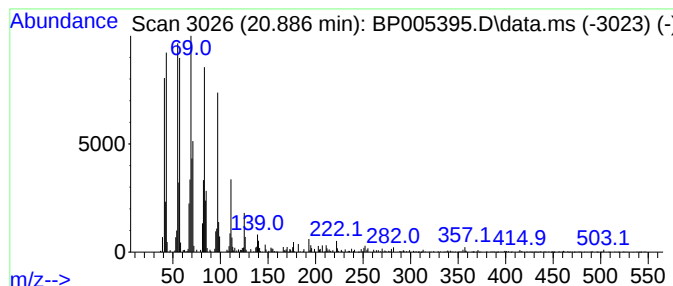
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Peak Number 4 Bromoacetic acid, octadecyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.886	5.11 ng	132368	Chrysene-d12	21.175	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2	9-Octadecene, (E)-	252	C18H36	007206-25-9	89
3	1-Octadecene	252	C18H36	000112-88-9	86
4	Octacosyl acetate	452	C30H60O2	018206-97-8	78
5	13-Methyl-Z-14-nonacosene	420	C30H60	1000131-19-0	78



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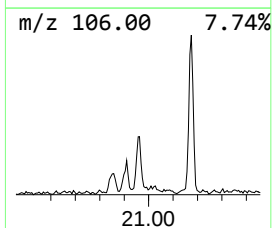
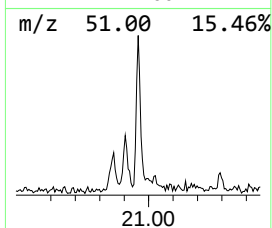
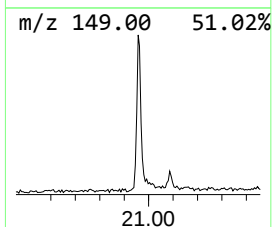
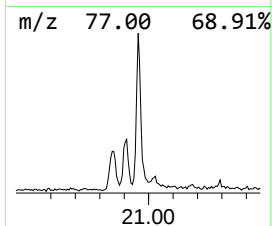
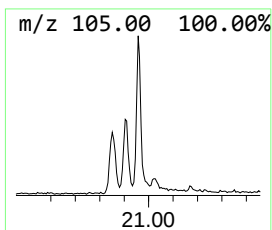
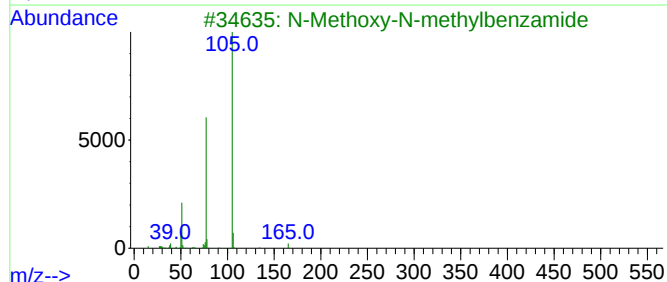
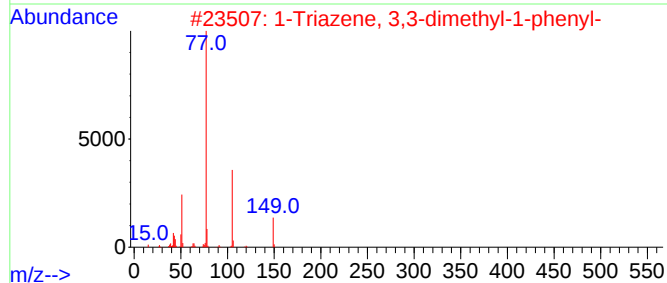
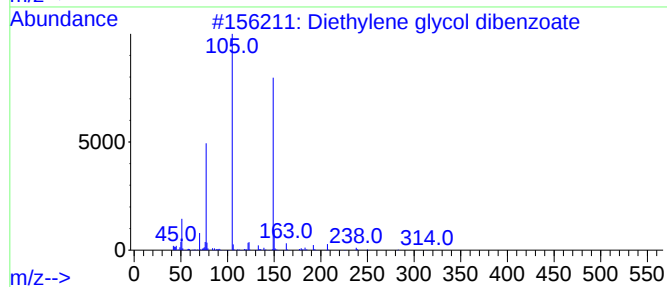
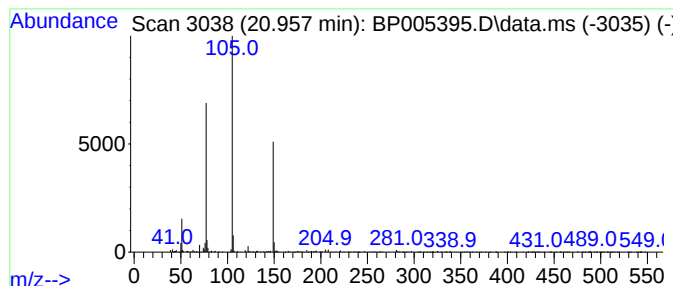
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.957	3.56 ng	92409	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	72
2			1-Triazene, 3,3-dimethyl-1-phenyl-	149	C8H11N3	007227-91-0	72
3			N-Methoxy-N-methylbenzamide	165	C9H11NO2	006919-61-5	38
4			1,3,4-Oxadiazin-6-one, 5-isoprop...	216	C12H12N2O2	173973-78-9	38
5			Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Tridecanoic acid	17.975	10.7	ng	180548	4	17.069	337588	20.0
Octadecanoic acid	19.216	3.7	ng	96706	5	21.175	518427	20.0
Bromoacetic aci...	20.886	5.1	ng	132368	5	21.175	518427	20.0
Diethylene glyc...	20.957	3.6	ng	92409	5	21.175	518427	20.0