

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092623\
 Data File : BF135462.D
 Acq On : 26 Sep 2023 20:00
 Operator : CG\JU
 Sample : 04566-06 2X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B102-08-1

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-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135462.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.781	284	288	294	rVB2	9271	14819	1.09%	0.111%
2	5.387	557	561	577	rBV	1253886	1361450	100.00%	10.178%
3	6.398	730	733	749	rBV	1331134	1346163	98.88%	10.064%
4	6.757	790	794	800	rBV	886121	841011	61.77%	6.287%
5	7.316	886	889	901	rBV	908584	793738	58.30%	5.934%
6	8.034	1007	1011	1016	rBV	1181841	972380	71.42%	7.269%
7	9.110	1190	1194	1197	rBV	1462440	1157736	85.04%	8.655%
8	9.228	1211	1214	1219	rBV	21228	22481	1.65%	0.168%
9	9.786	1306	1309	1313	rBV	1001455	905942	66.54%	6.773%
10	9.998	1340	1345	1349	rBV6	8829	15663	1.15%	0.117%
11	10.580	1441	1444	1455	rBV	680328	634290	46.59%	4.742%
12	11.280	1559	1563	1567	rBV	1056076	932344	68.48%	6.970%
13	11.680	1627	1631	1635	rBV2	17108	16750	1.23%	0.125%
14	11.816	1651	1654	1658	rBV	181351	189134	13.89%	1.414%
15	12.504	1769	1771	1774	rBV	27699	26178	1.92%	0.196%
16	12.610	1786	1789	1794	rBV5	26801	35331	2.60%	0.264%
17	12.733	1808	1810	1812	rBV	24394	16653	1.22%	0.124%
18	12.874	1830	1834	1838	rBV	1206875	1020353	74.95%	7.628%
19	13.110	1872	1874	1878	rBV2	18683	14172	1.04%	0.106%
20	13.363	1914	1917	1924	rBV	185864	183969	13.51%	1.375%
21	13.421	1924	1927	1930	rBV	132385	110922	8.15%	0.829%
22	13.557	1947	1950	1952	rBV	100057	86529	6.36%	0.647%
23	13.592	1953	1956	1960	rVV	1221990	1159060	85.13%	8.665%
24	13.921	2009	2012	2013	rBV	299450	279666	20.54%	2.091%
25	13.939	2013	2015	2019	rVB	819643	682422	50.12%	5.102%
26	15.410	2261	2265	2271	rVB	438302	557453	40.95%	4.167%

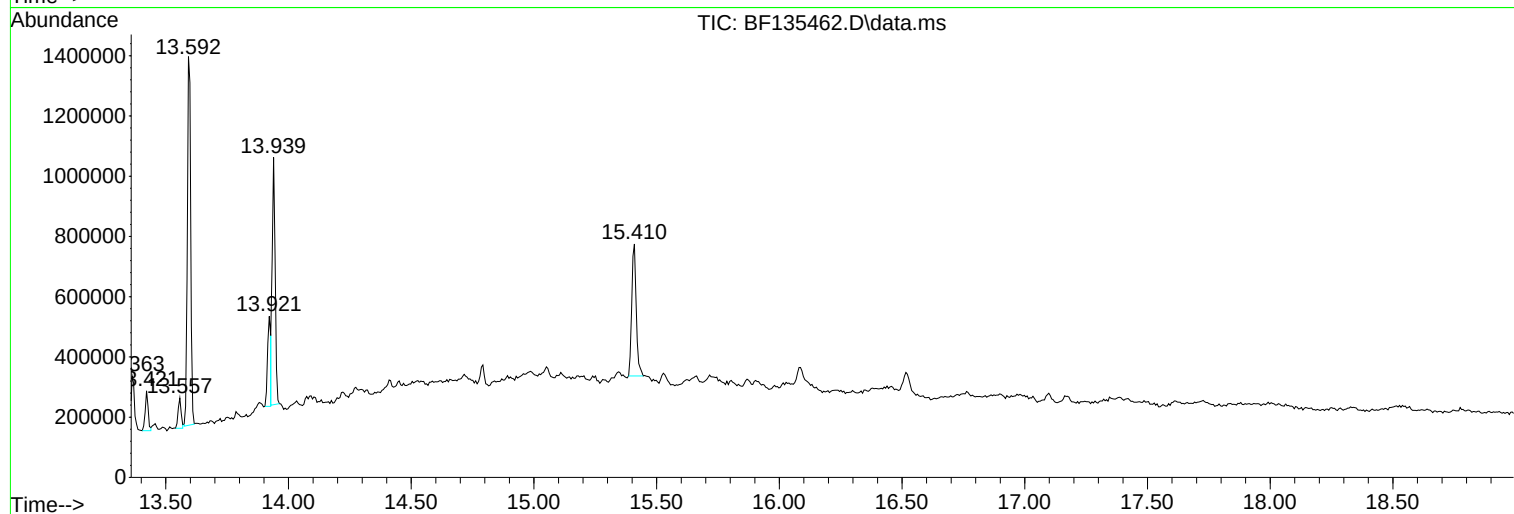
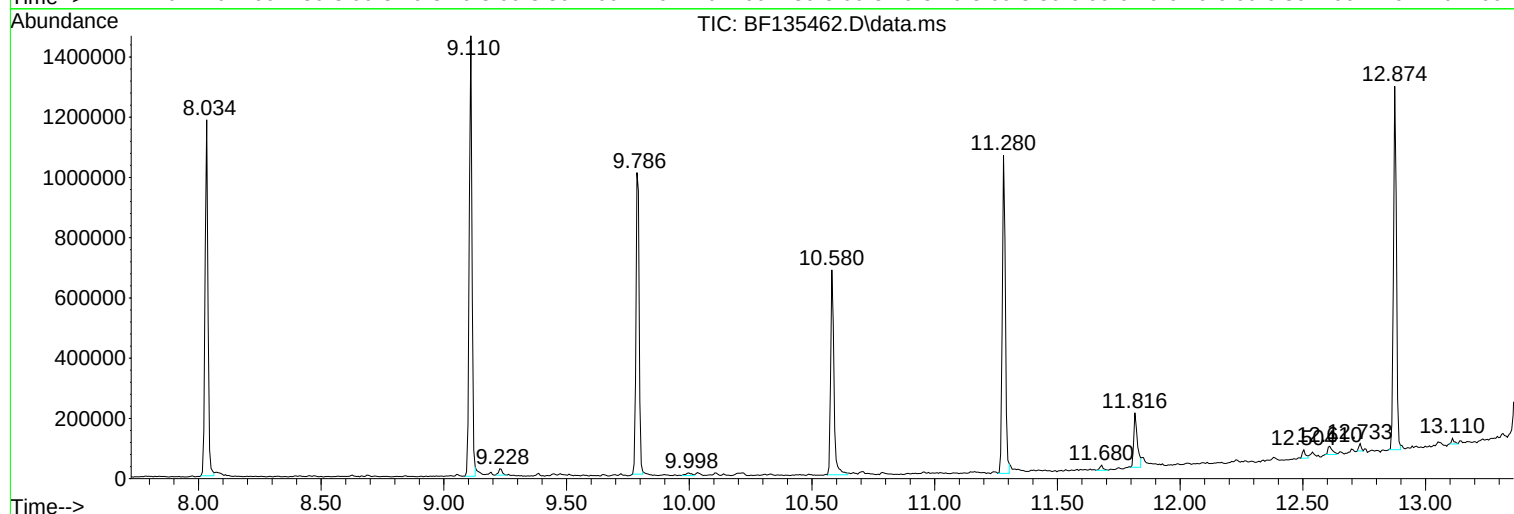
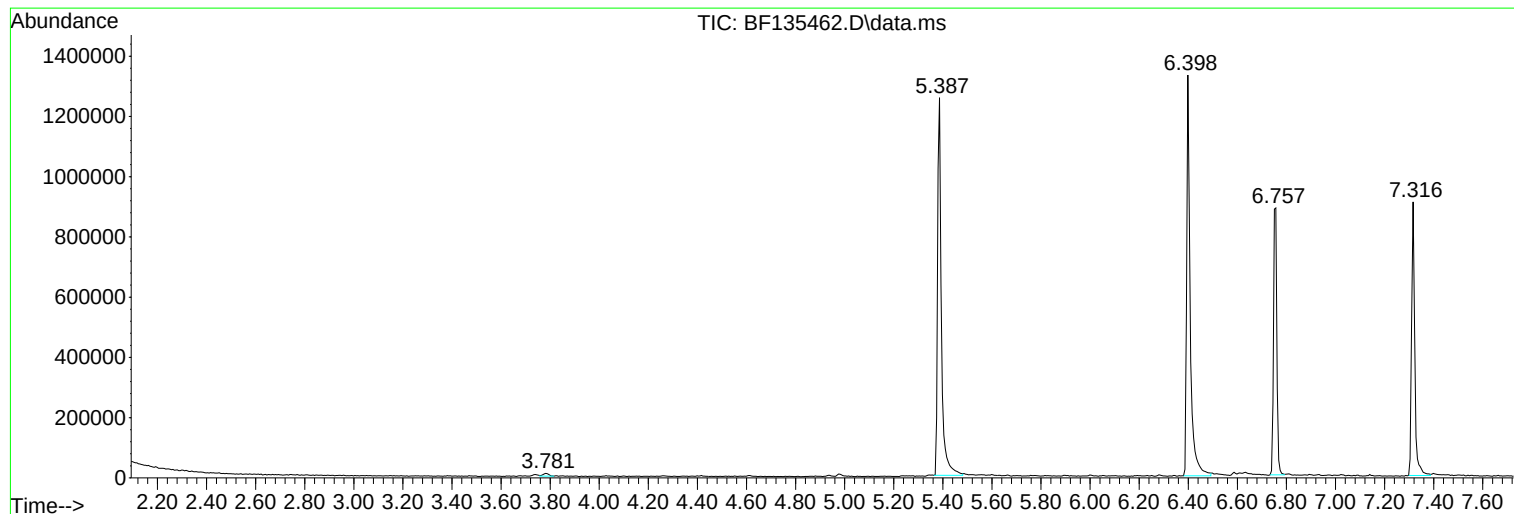
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ClientSampleId :
B102-08-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.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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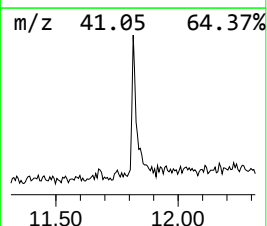
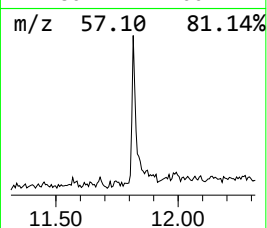
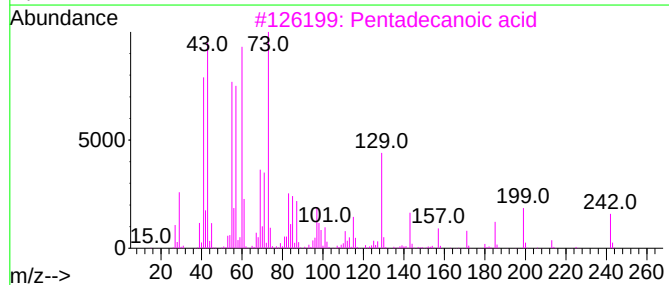
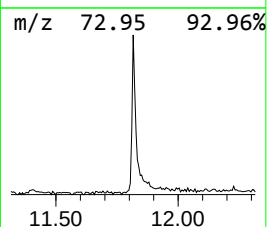
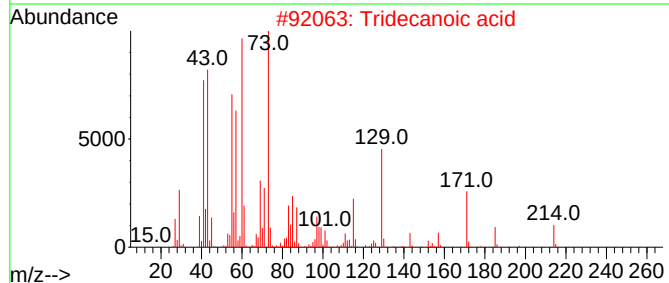
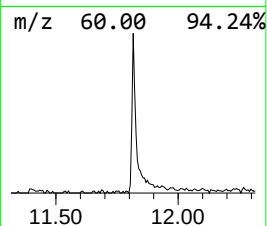
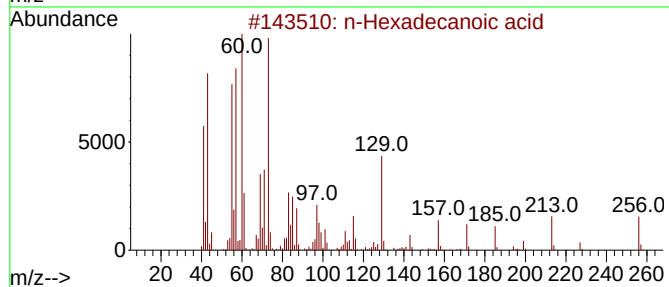
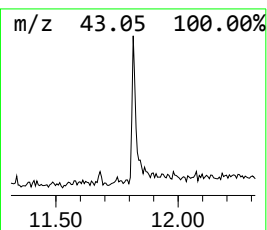
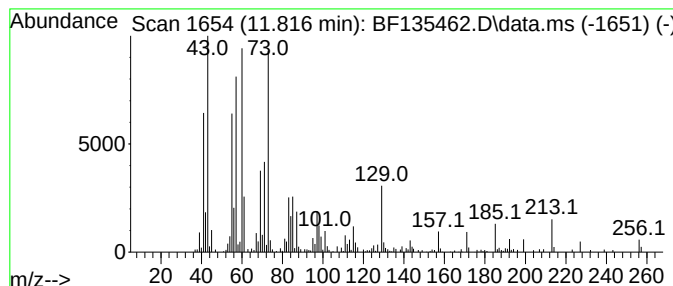
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.816	4.06 ng	189134	Phenanthrene-d10	11.280

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	89
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5			n-Decanoic acid	172	C10H20O2	000334-48-5	58



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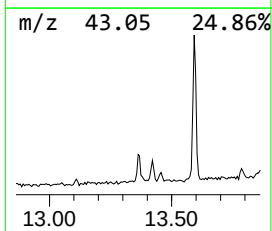
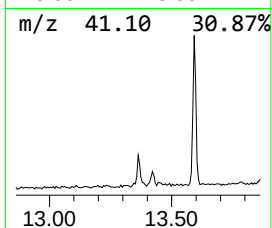
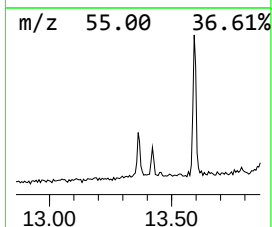
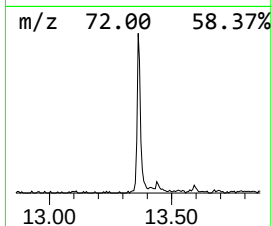
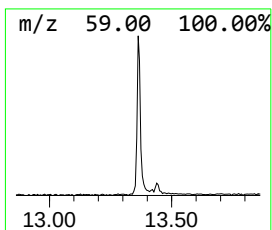
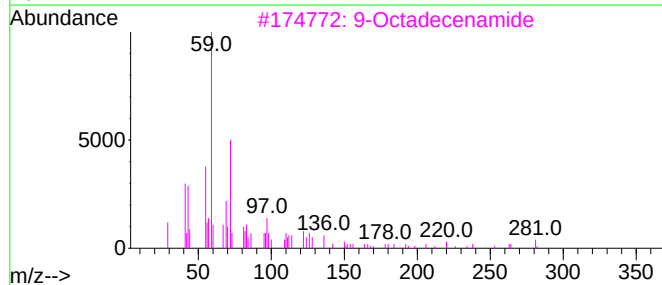
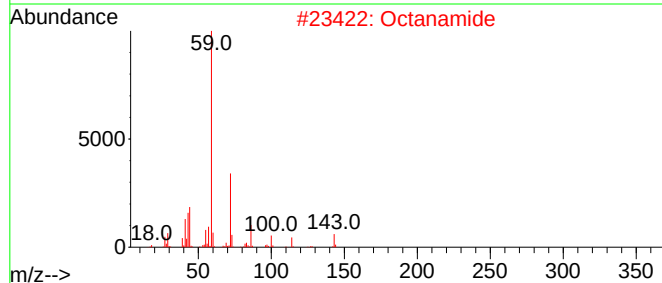
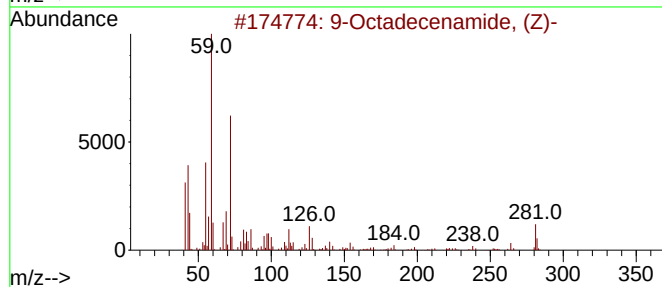
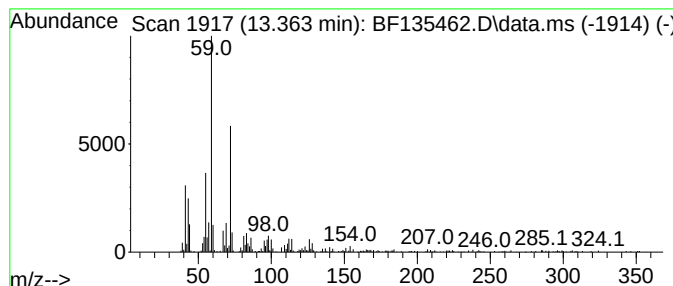
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Peak Number 2 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.363	5.39 ng	183969	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	93
2			Octanamide	143	C8H17NO	000629-01-6	78
3			9-Octadecenamide	281	C18H35NO	003322-62-1	78
4			Pentadecanamide, 15-bromo-	319	C15H30BrNO	1000163-86-1	64
5			Nonanamide	157	C9H19NO	001120-07-6	59



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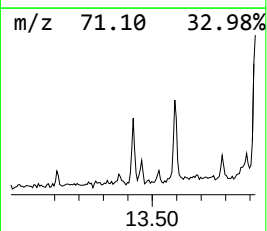
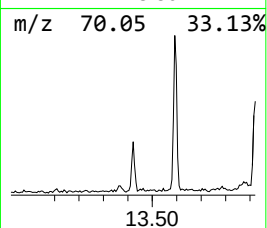
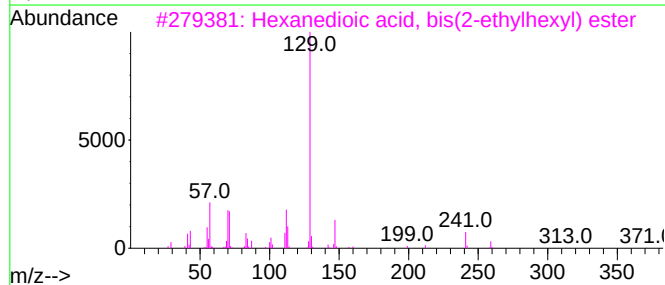
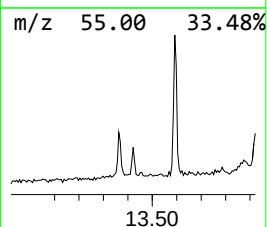
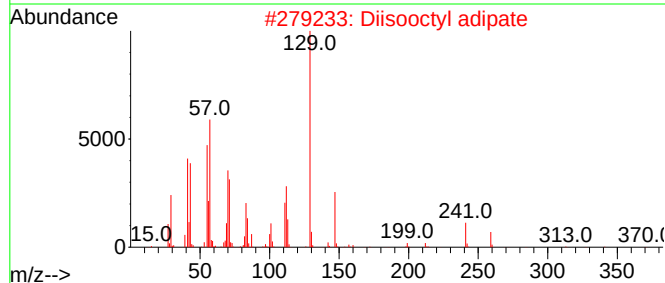
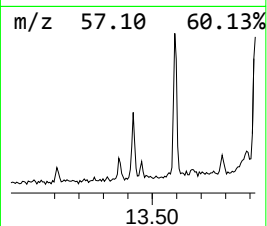
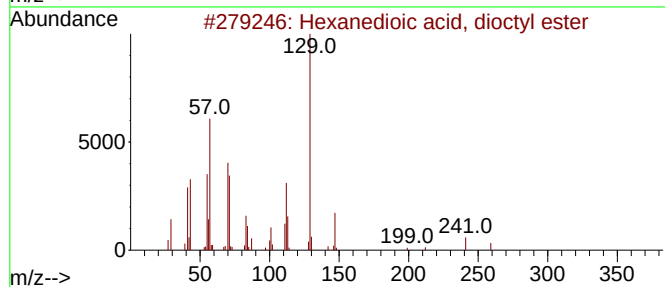
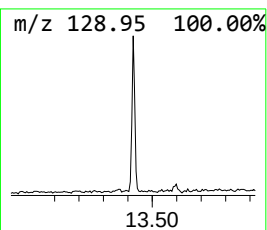
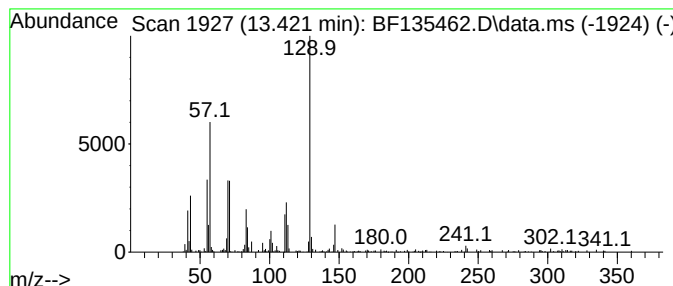
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexanedioic acid, dioctyl e... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.422	3.25 ng	110922	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanedioic acid, dioctyl ester	370	C22H42O4	000123-79-5	91
2			Diisooctyl adipate	370	C22H42O4	001330-86-5	90
3			Hexanedioic acid, bis(2-ethylhex...	370	C22H42O4	000103-23-1	90
4			Hexanedioic acid, mono(2-ethylhe...	258	C14H26O4	004337-65-9	58
5			Adipic acid, 2-ethylhexyl isohex...	342	C20H38O4	1000324-48-3	50



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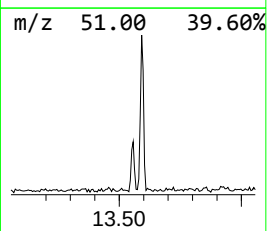
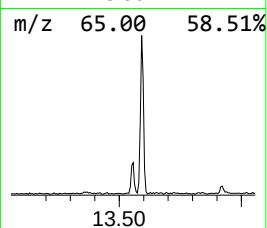
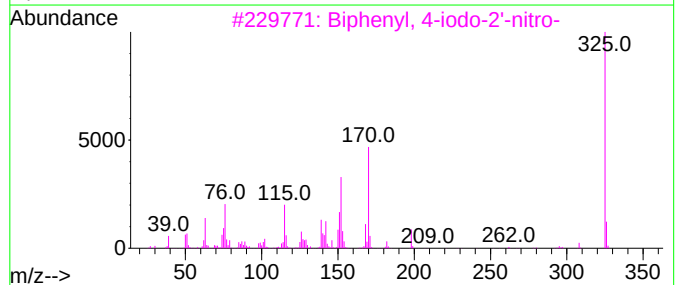
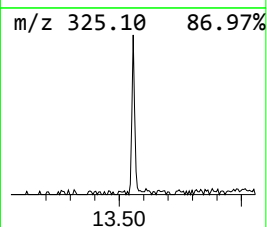
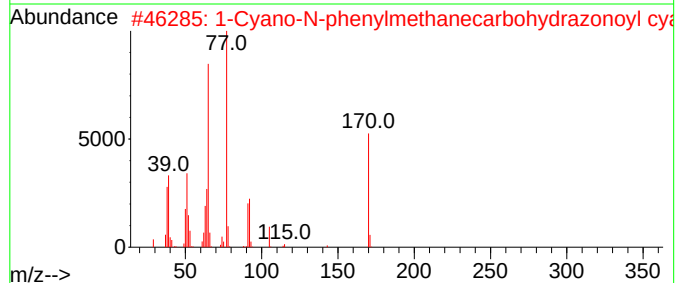
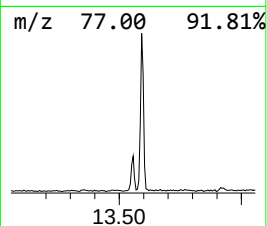
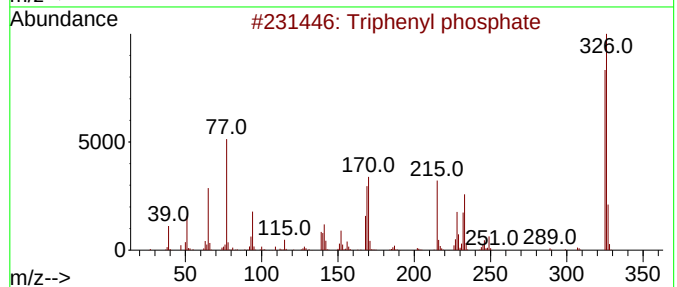
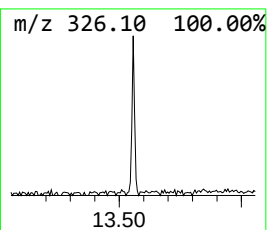
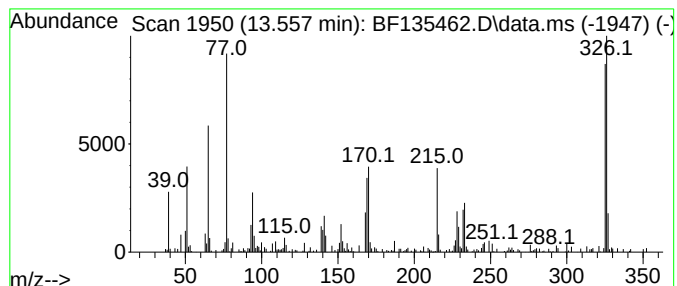
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Triphenyl phosphate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.557	2.54 ng	86529	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Triphenyl phosphate	326	C18H15O4P	000115-86-6	96
2			1-Cyano-N-phenylmethanecarbohydr...	170	C9H6N4	000306-18-3	32
3			Biphenyl, 4-iodo-2'-nitro-	325	C12H8IN02	002499-77-6	15
4			2-Methyl-3,8-diphenyl-3H-imidazo...	325	C21H15N3O	089174-96-9	14
5			N-(2-Cyano-ethyl)-benzenesulfona...	210	C9H10N2O2S	002619-21-8	11



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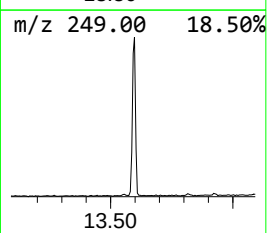
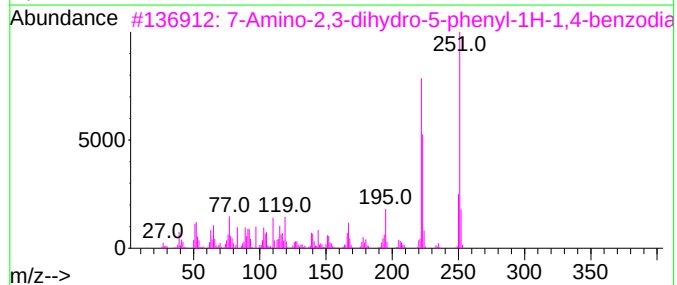
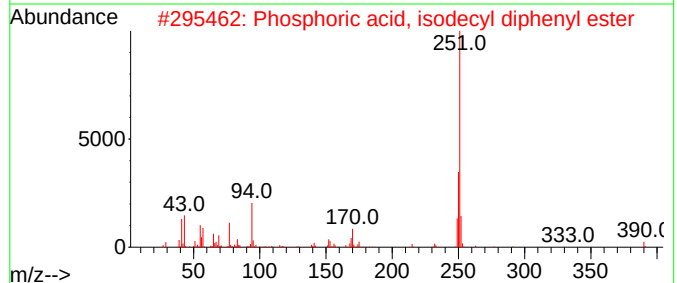
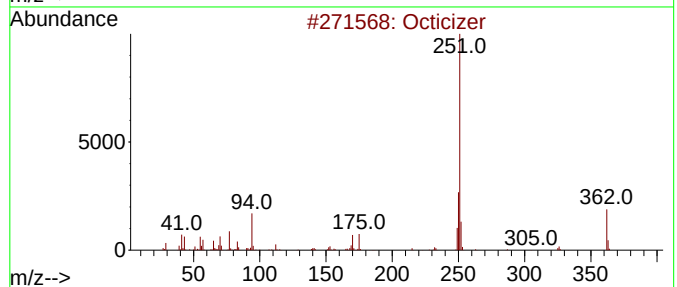
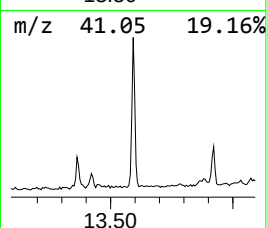
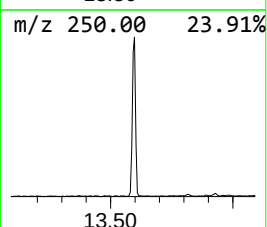
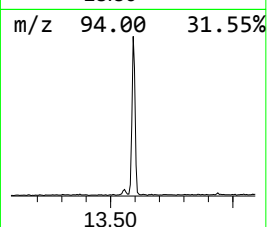
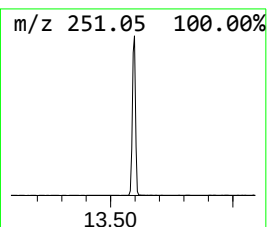
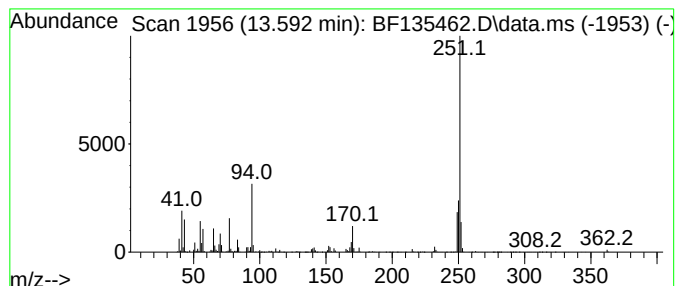
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octicizer Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.592	33.97 ng	1159060	Chrysene-d12	13.939

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octicizer	362	C20H27O4P	001241-94-7	95
2			Phosphoric acid, isodecyl diphen...	390	C22H31O4P	1346599-15-2	87
3			7-Amino-2,3-dihydro-5-phenyl-1H-...	251	C15H13N3O	004928-02-3	53
4			2-Benzo[1,3]dioxol-5-yl-7-methyl...	251	C16H13NO2	1000274-75-9	50
5			2H-1,3,4-Benzotriazepin-2-one, 1...	251	C15H13N3O	002855-57-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.816	4.1	ng	189134	4	11.280	932344	20.0
9-Octadecenamid...	13.363	5.4	ng	183969	5	13.939	682422	20.0
Hexanedioic aci...	13.422	3.3	ng	110922	5	13.939	682422	20.0
Triphenyl phosph...	13.557	2.5	ng	86529	5	13.939	682422	20.0
Octicizer	13.592	34.0	ng	1159060	5	13.939	682422	20.0