

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042623\
 Data File : BF133078.D
 Acq On : 26 Apr 2023 22:04
 Operator : CG\JU
 Sample : 02448-08
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20230346-COMP-24

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF133078.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.934	481	484	491	rVB	59481	79388	1.62%	0.218%
2	5.345	549	554	557	rBV	4522017	4770043	97.38%	13.112%
3	6.375	723	729	732	rBV	4387493	4751807	97.01%	13.062%
4	6.733	786	790	793	rBV	1374240	1021062	20.85%	2.807%
5	7.298	881	886	889	rBV	3225442	2956927	60.37%	8.128%
6	8.016	1005	1008	1011	rBV	1775878	1420261	29.00%	3.904%
7	9.098	1187	1192	1195	rBV	5332265	4820382	98.41%	13.251%
8	9.769	1302	1306	1309	rBV	2116065	1605786	32.78%	4.414%
9	10.480	1424	1427	1431	rVB	487329	382491	7.81%	1.051%
10	10.557	1435	1440	1443	rBV	3449236	3201185	65.35%	8.800%
11	11.251	1554	1558	1560	rBV	1875670	1668551	34.06%	4.587%
12	11.268	1560	1561	1564	rVV	113910	88427	1.81%	0.243%
13	11.321	1568	1570	1573	rVB	98627	79087	1.61%	0.217%
14	11.786	1645	1649	1653	rBV	590227	532271	10.87%	1.463%
15	12.457	1760	1763	1766	rBV	132314	112535	2.30%	0.309%
16	12.568	1780	1782	1787	rBV	70480	66048	1.35%	0.182%
17	12.686	1797	1802	1805	rBV	106016	117350	2.40%	0.323%
18	12.839	1824	1828	1831	rBV	5222197	4898271	100.00%	13.465%
19	13.015	1855	1858	1861	rVB	70679	63507	1.30%	0.175%
20	13.080	1866	1869	1872	rVV	92435	75481	1.54%	0.207%
21	13.421	1924	1927	1933	rBV3	61779	69581	1.42%	0.191%
22	13.651	1964	1966	1975	rVB5	56444	88953	1.82%	0.245%
23	13.804	1987	1992	1998	rBV4	124045	205763	4.20%	0.566%
24	13.880	2000	2005	2008	rVV	1419078	1393991	28.46%	3.832%
25	13.904	2008	2009	2017	rVB	149817	125218	2.56%	0.344%
26	14.068	2032	2037	2040	rBV2	42502	53066	1.08%	0.146%
27	14.739	2147	2151	2155	rBV	534452	515355	10.52%	1.417%
28	14.892	2174	2177	2180	rBV	52394	74462	1.52%	0.205%
29	15.239	2233	2236	2240	rVB	54080	58395	1.19%	0.161%
30	15.304	2242	2247	2253	rBV	940271	1082499	22.10%	2.976%

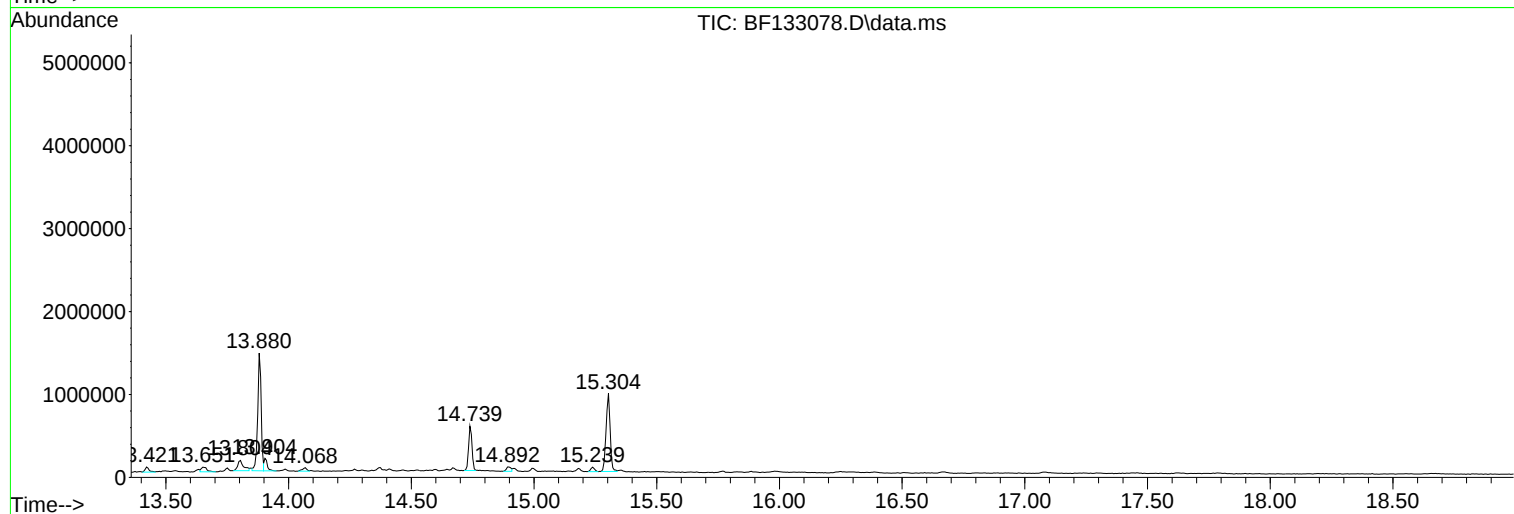
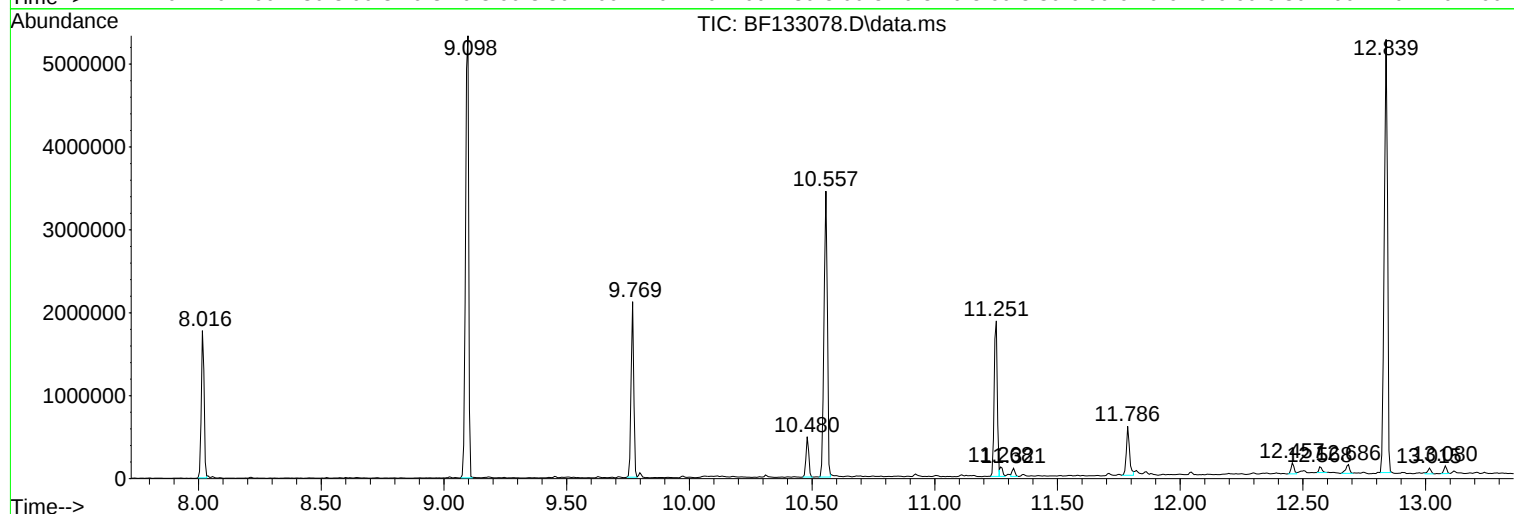
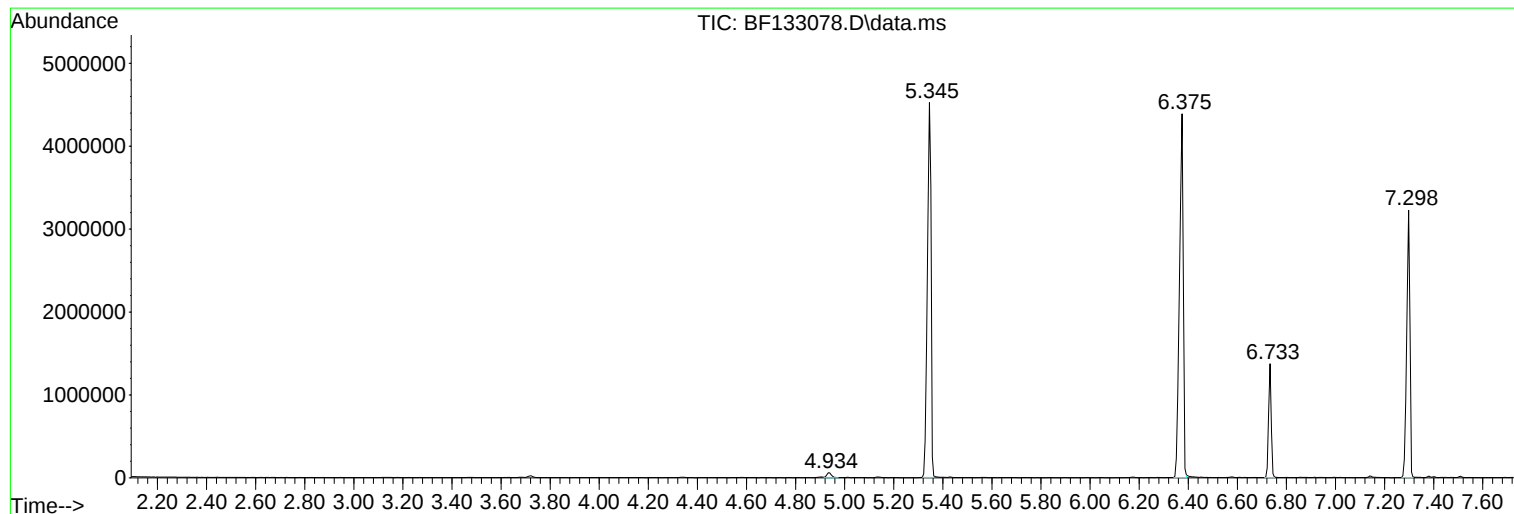
Sum of corrected areas: 36378143

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.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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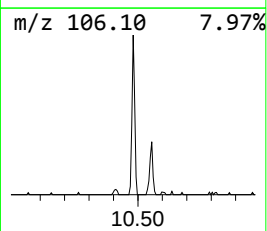
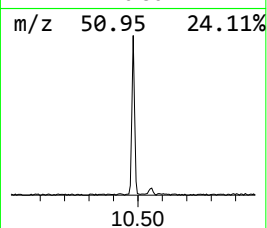
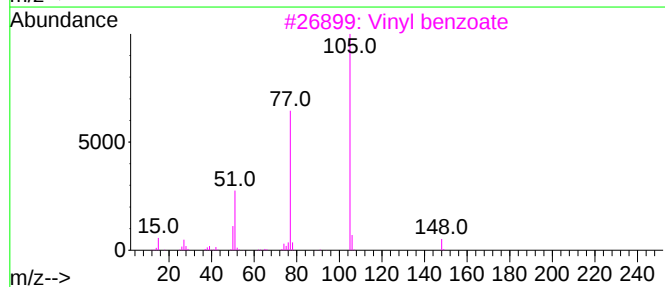
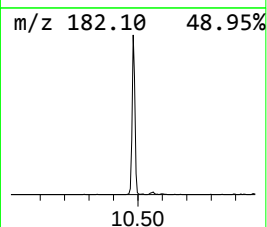
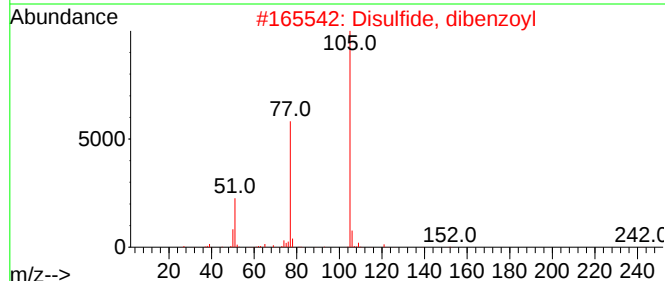
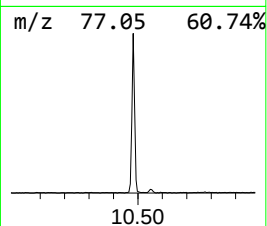
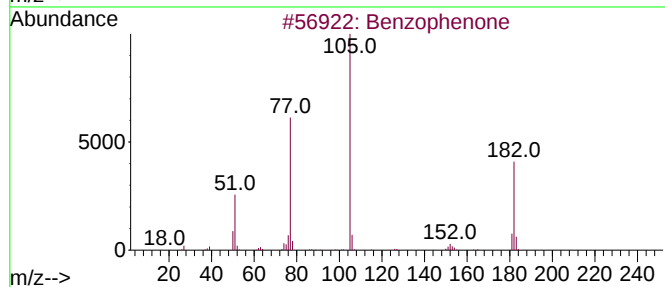
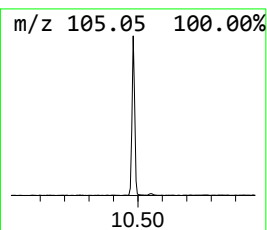
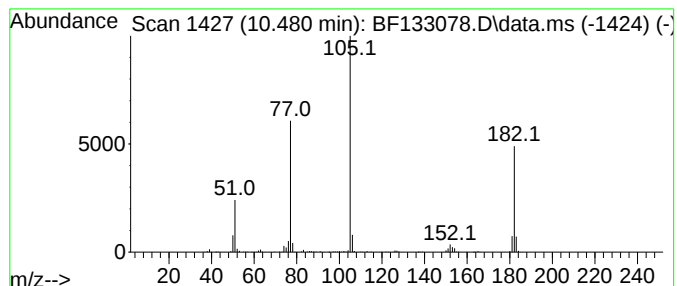
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.480	4.76 ng	382491	Acenaphthene-d10	9.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Disulfide, dibenzoyl	274	C14H10O2S2	000644-32-6	49
3			Vinyl benzoate	148	C9H8O2	000769-78-8	47
4			2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47
5			1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47



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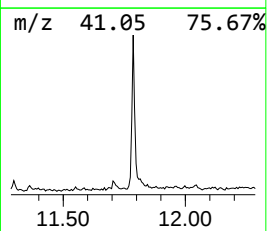
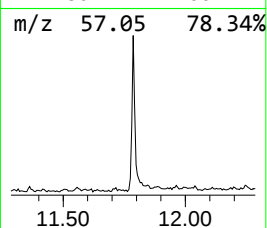
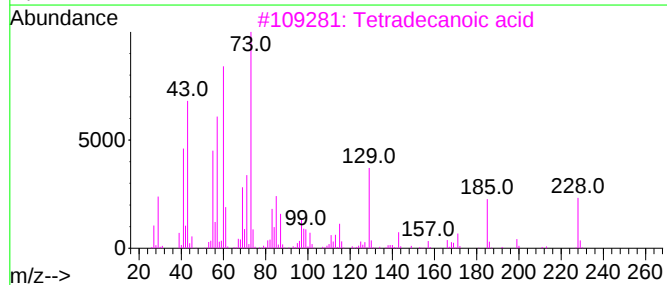
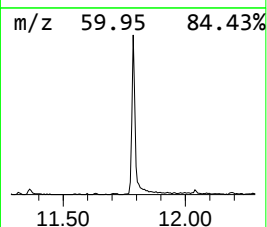
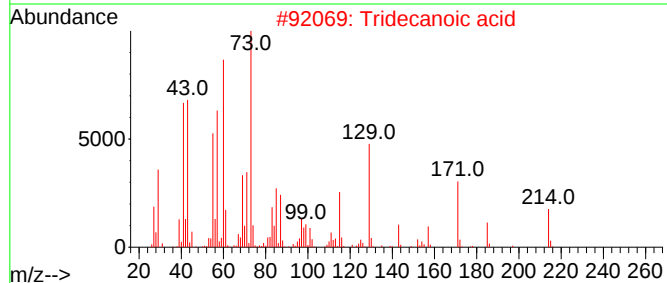
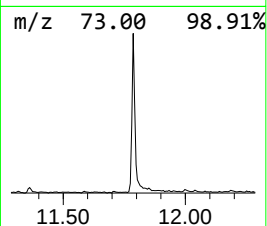
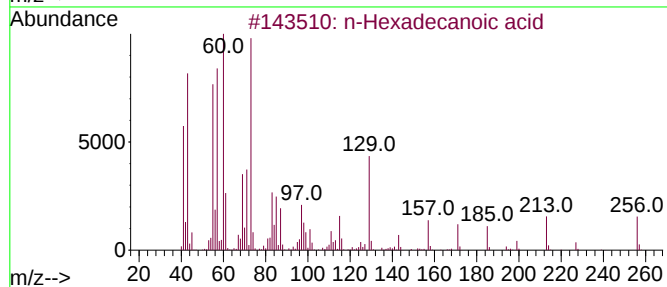
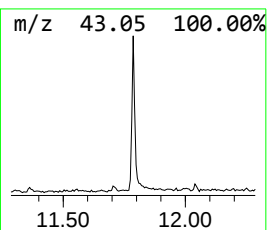
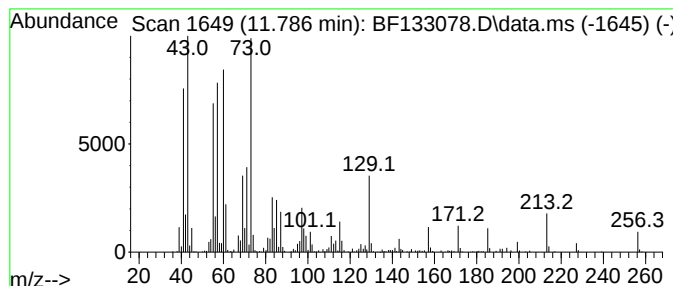
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.786	6.38 ng	532271	Phenanthrene-d10	11.251

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	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	49



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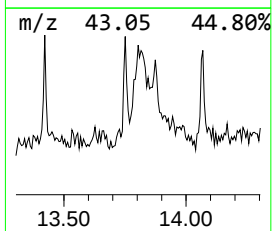
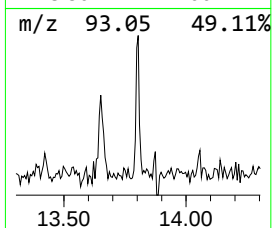
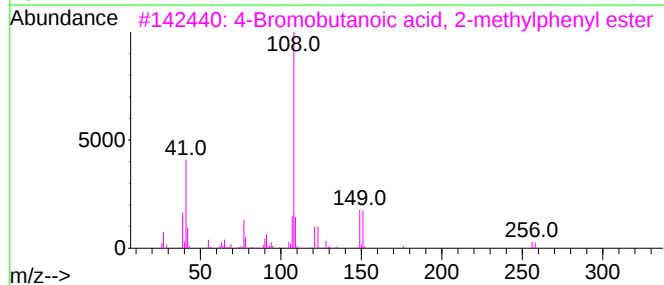
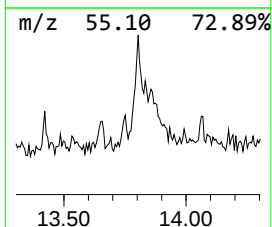
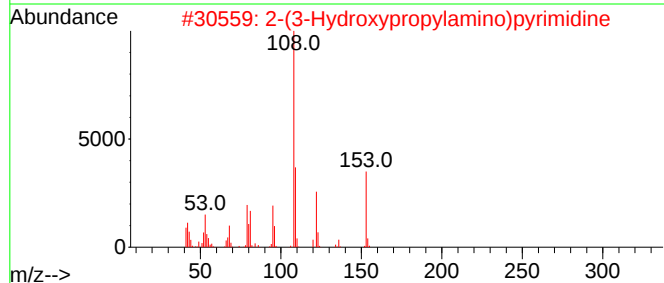
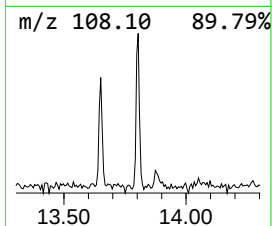
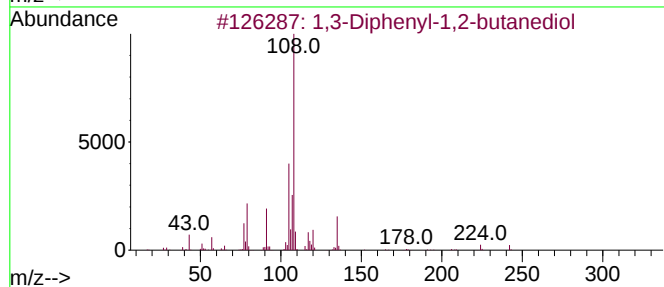
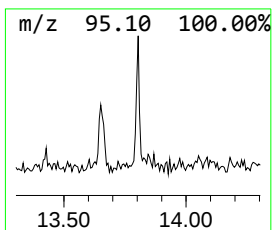
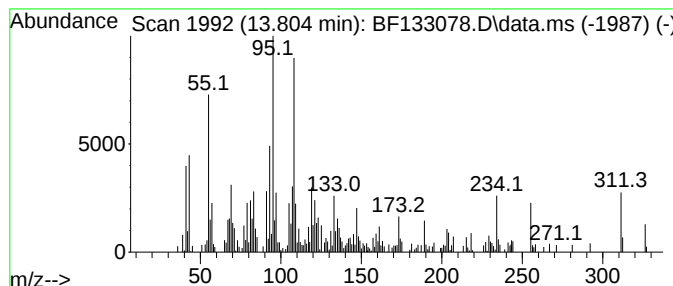
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 unknown13.804 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.804	2.95 ng	205763	Chrysene-d12	13.880

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Diphenyl-1,2-butanediol	242	C16H18O2	005381-88-4	35
2			2-(3-Hydroxypropylamino)pyrimidine	153	C7H11N3O	1000255-82-5	22
3			4-Bromobutanoic acid, 2-methylph...	256	C11H13BrO2	1010293-67-3	18
4			Urea, N-(6-methyl-2-pyridinyl)-N...	241	C14H15N3O	1000350-96-6	15
5			Benzofuran, 6-ethenyl-4,5,6,7-te...	216	C15H20O	017910-09-7	14



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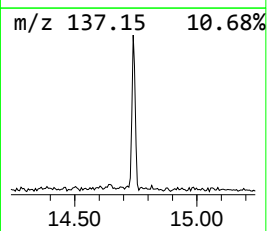
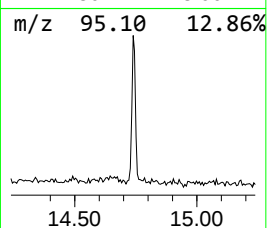
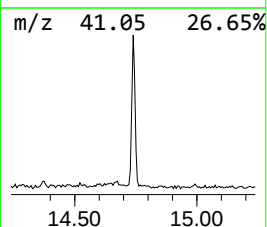
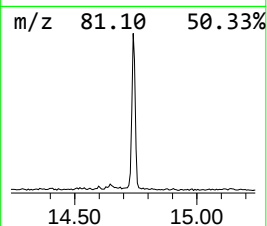
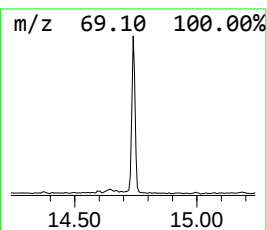
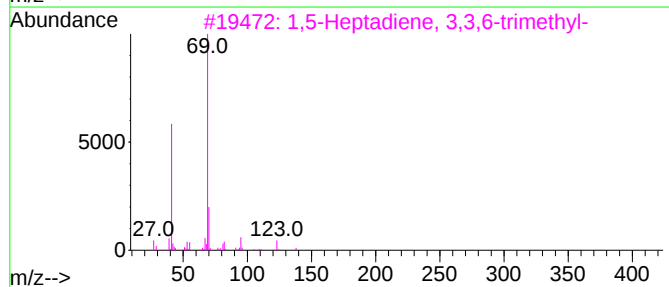
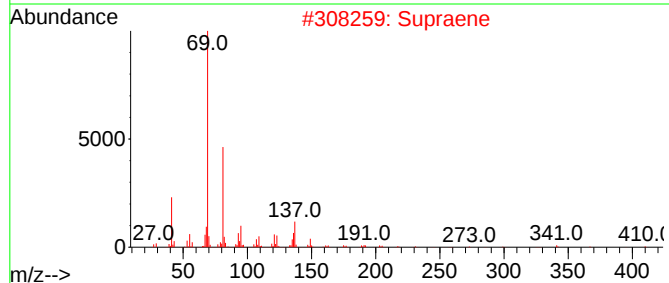
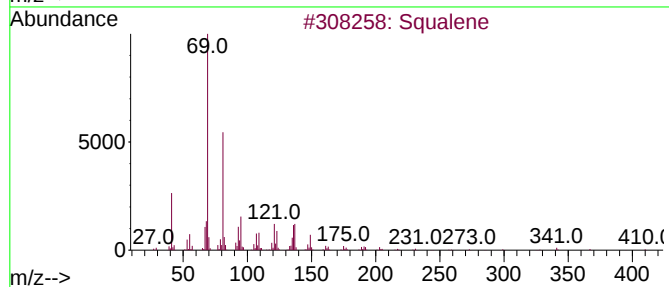
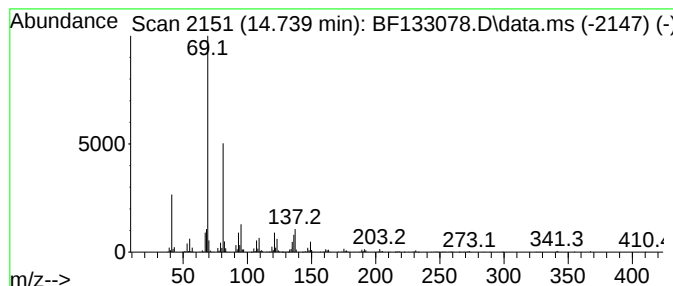
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Peak Number 4 Squalene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.739	9.52 ng	515355	Perylene-d12	15.304

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	95
2			Supraene	410	C30H50	007683-64-9	91
3			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	52
4			1,6-Octadiene, 3,5-dimethyl-, tr...	138	C10H18	074630-87-8	50
5			2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzophenone	10.480	4.8	ng	382491	3	9.769	1605790	20.0
n-Hexadecanoic ...	11.786	6.4	ng	532271	4	11.251	1668550	20.0
unknown13.804	13.804	3.0	ng	205763	5	13.880	1393990	20.0
Squalene	14.739	9.5	ng	515355	6	15.304	1082500	20.0