

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG100920\
 Data File : BG046837.D
 Acq On : 9 Oct 2020 17:03
 Operator : CG/JU
 Sample : L4303-21
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 IDW-20201006

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_G\METHODS\8270-BG092220.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG046837.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.665	388	396	405	rBV	907327	1459548	34.06%	7.120%
2	7.257	659	667	680	rBV	908718	1579789	36.87%	7.706%
3	8.103	804	811	819	rBV	222991	386940	9.03%	1.887%
4	9.267	1001	1009	1018	rVB	613184	1082137	25.25%	5.279%
5	10.918	1282	1290	1298	rBV	293379	525377	12.26%	2.563%
6	13.356	1696	1705	1712	rBV	1543717	2386687	55.70%	11.642%
7	14.173	1838	1844	1852	rBV	98190	146528	3.42%	0.715%
8	14.725	1931	1938	1946	rBV	462476	730567	17.05%	3.564%
9	16.211	2183	2191	2201	rBV	1239511	1891791	44.15%	9.228%
10	16.546	2243	2248	2253	rBV	40235	59180	1.38%	0.289%
11	16.605	2253	2258	2264	rVB3	45183	84313	1.97%	0.411%
12	16.664	2264	2268	2272	rBV2	41726	58785	1.37%	0.287%
13	16.770	2280	2286	2290	rBV3	42856	76302	1.78%	0.372%
14	16.870	2297	2303	2308	rBV5	40075	80074	1.87%	0.391%
15	16.934	2310	2314	2317	rBV	33355	47107	1.10%	0.230%
16	17.469	2398	2405	2416	rBV	628143	946668	22.09%	4.618%
17	18.350	2550	2555	2565	rBV	222940	339486	7.92%	1.656%
18	19.514	2748	2753	2759	rVB2	30557	57787	1.35%	0.282%
19	19.619	2766	2771	2775	rBV2	90664	130169	3.04%	0.635%
20	19.766	2792	2796	2802	rVB	97312	112239	2.62%	0.548%
21	19.884	2811	2816	2828	rVB	281463	448497	10.47%	2.188%
22	20.078	2842	2849	2856	rBV	3189278	4284931	100.00%	20.902%
23	20.806	2969	2973	2979	rVB3	70212	99130	2.31%	0.484%
24	21.388	3064	3072	3089	rBV2	269032	608109	14.19%	2.966%
25	21.746	3126	3133	3140	rVB2	703817	1188959	27.75%	5.800%
26	22.563	3268	3272	3275	rBV4	25756	43918	1.02%	0.214%
27	24.090	3527	3532	3540	rVB4	51705	105216	2.46%	0.513%
28	25.013	3678	3689	3704	rVB	418598	1239855	28.94%	6.048%
29	26.217	3888	3894	3896	rBV6	33146	57090	1.33%	0.278%
30	26.358	3910	3918	3930	rBV6	47579	198817	4.64%	0.970%
31	27.710	4145	4148	4155	rVB2	19535	44178	1.03%	0.216%

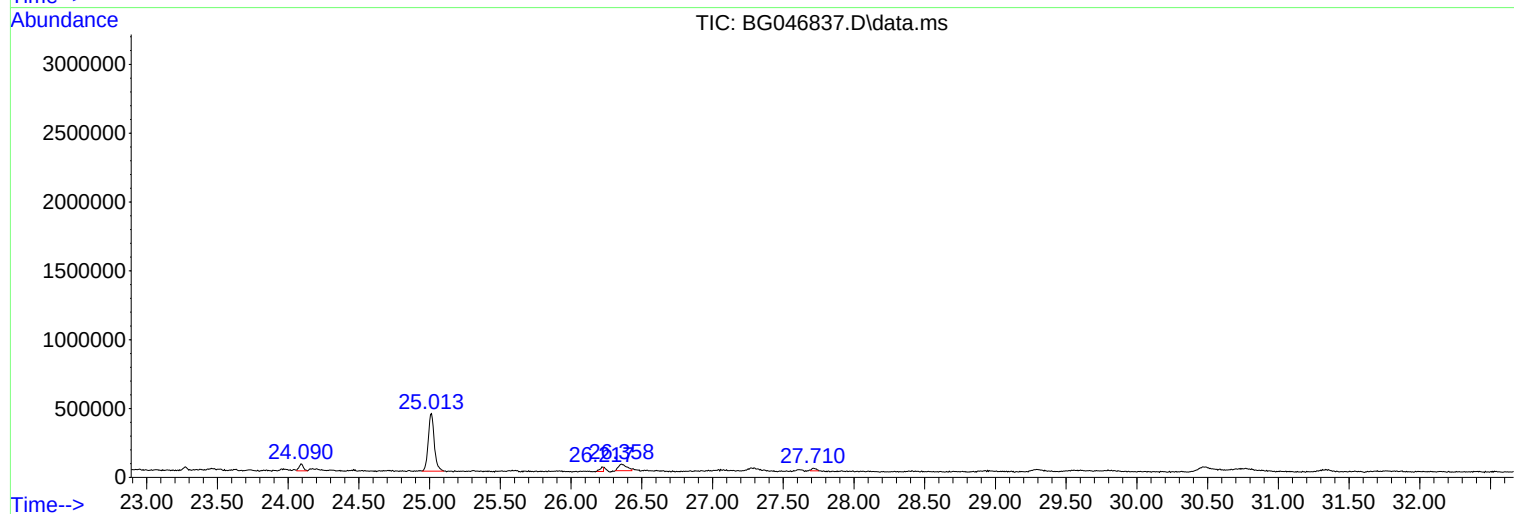
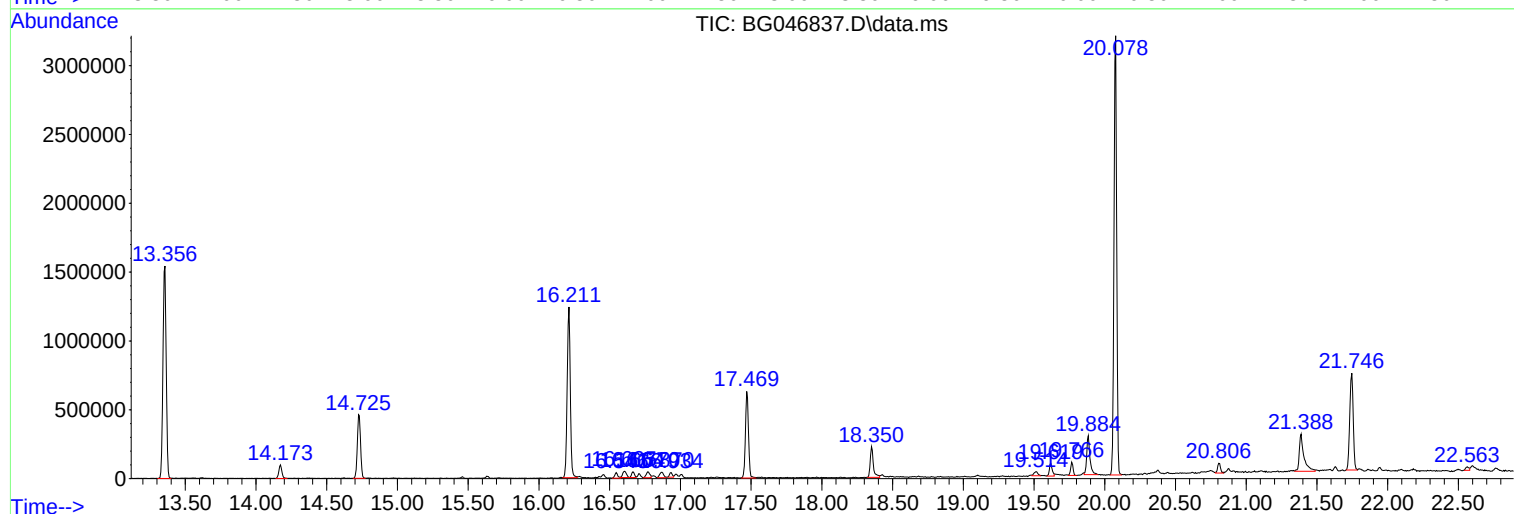
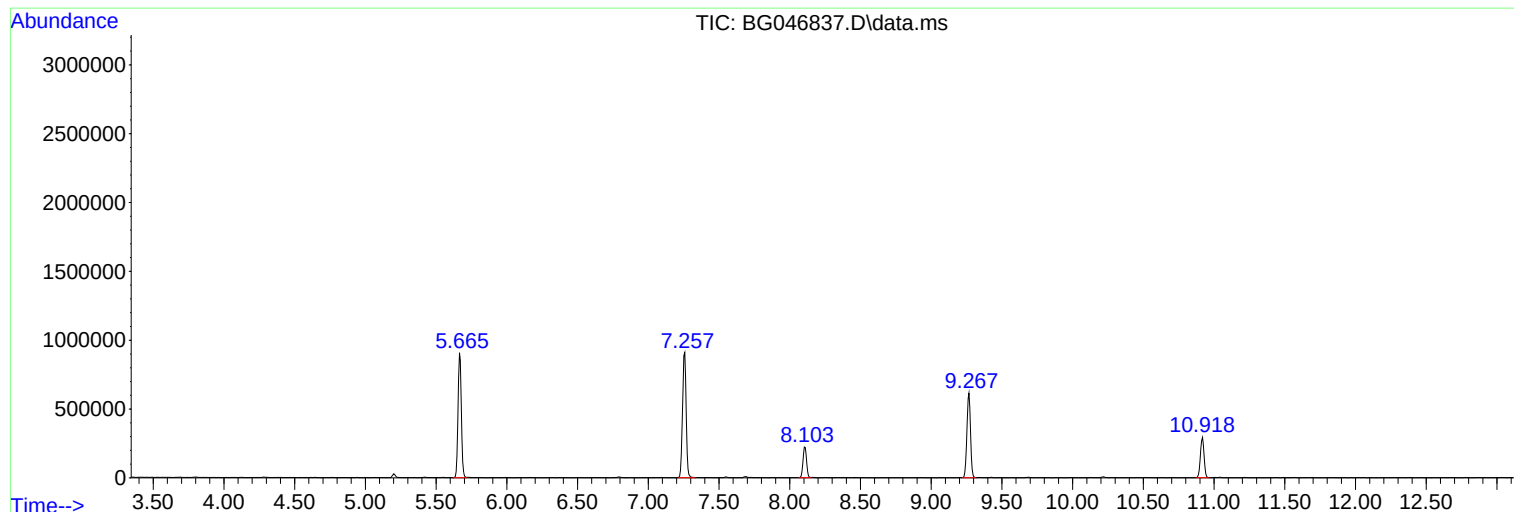
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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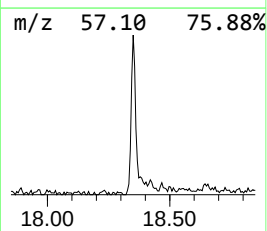
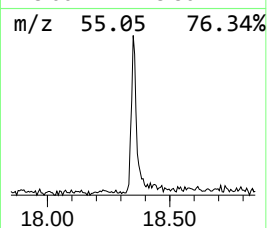
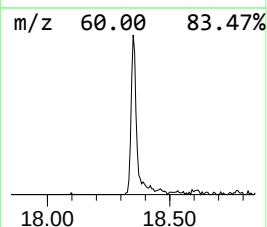
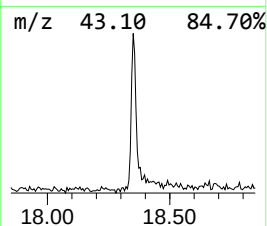
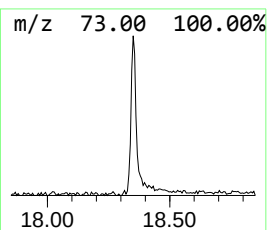
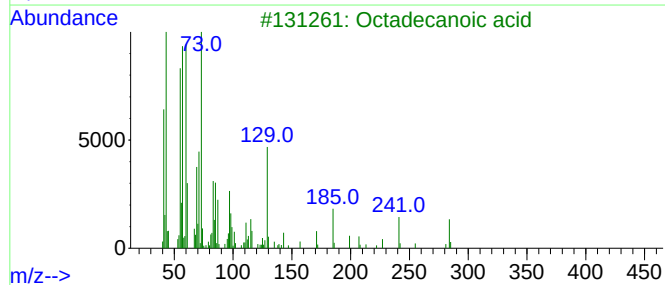
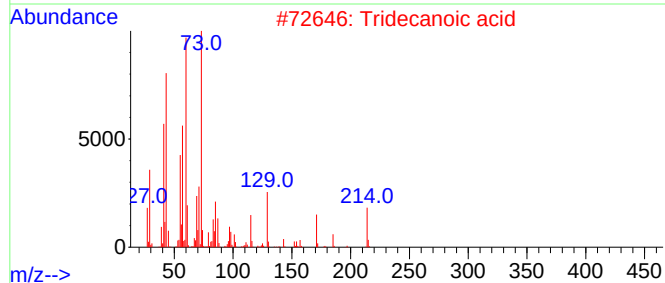
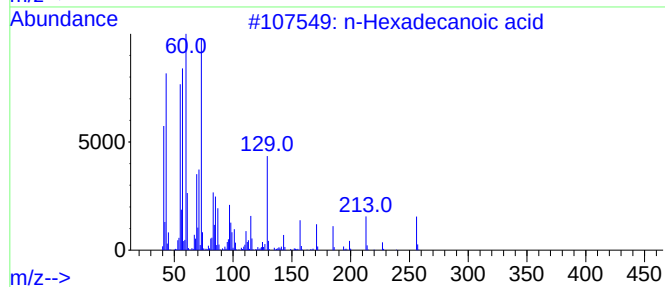
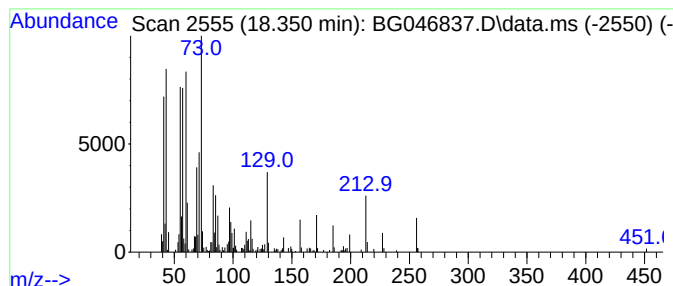
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.350	7.17 ng	339486	Phenanthrene-d10	17.469

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	93
3			Octadecanoic acid	284	C18H36O2	000057-11-4	81
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	72



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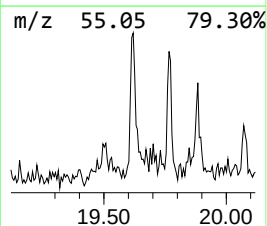
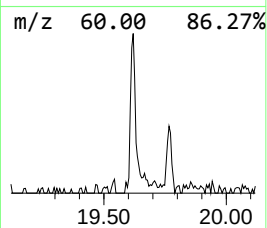
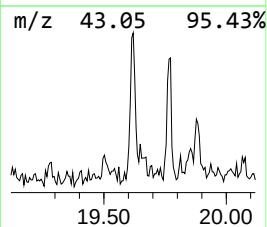
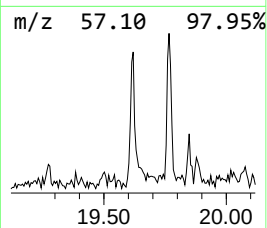
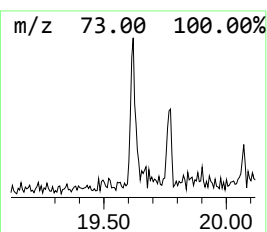
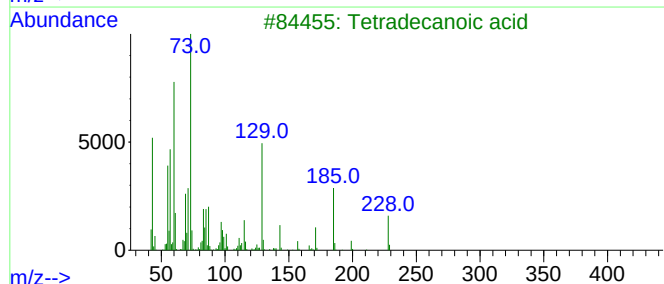
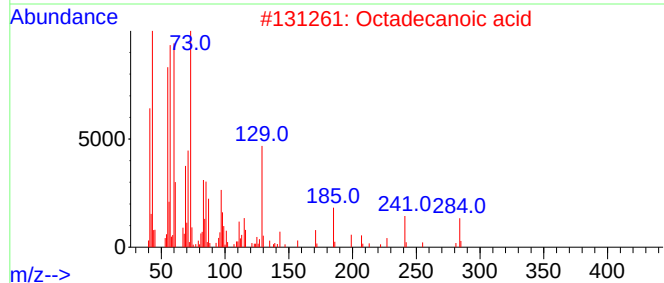
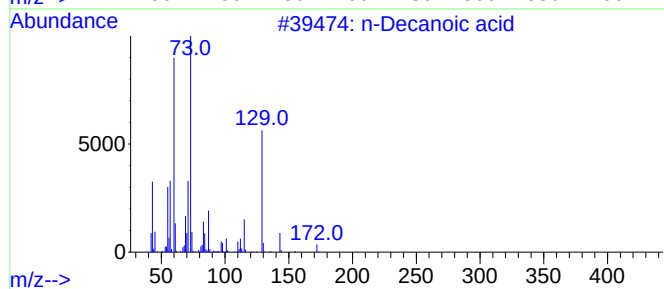
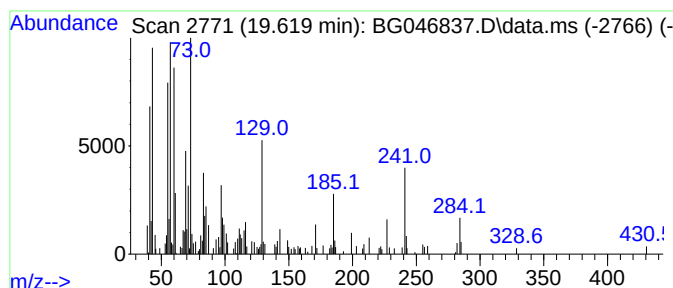
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
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Peak Number 2 n-Decanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.619	2.19 ng	130169	Chrysene-d12	21.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Decanoic acid	172	C10H20O2	000334-48-5	91
2			Octadecanoic acid	284	C18H36O2	000057-11-4	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	53
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



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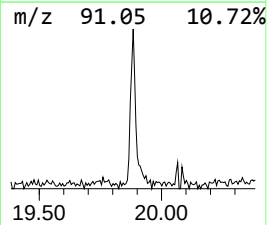
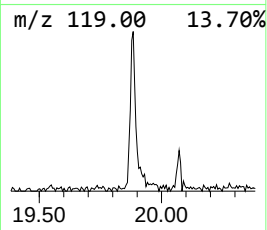
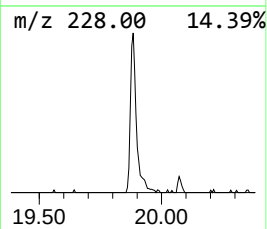
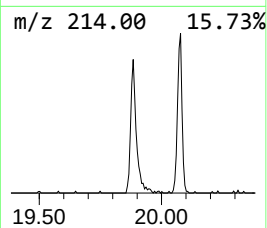
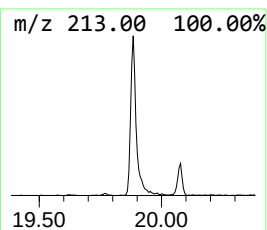
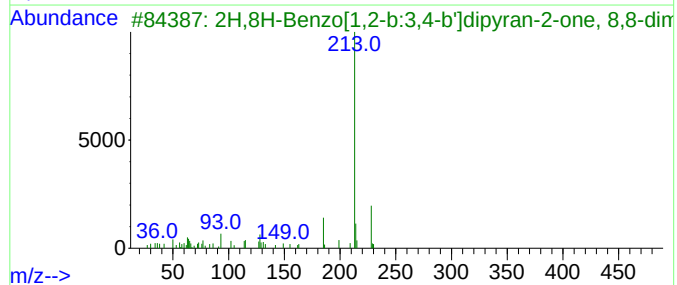
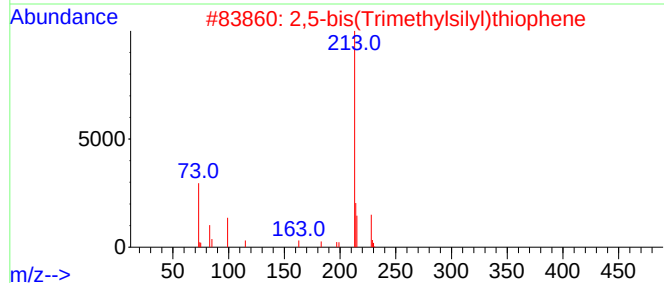
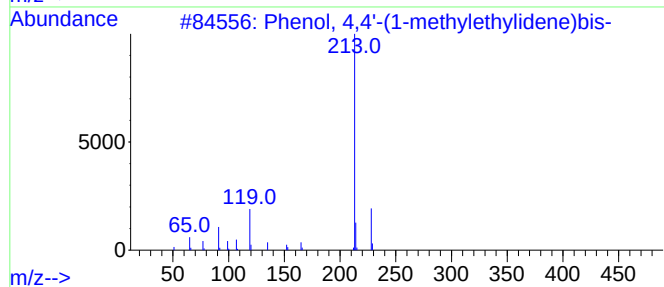
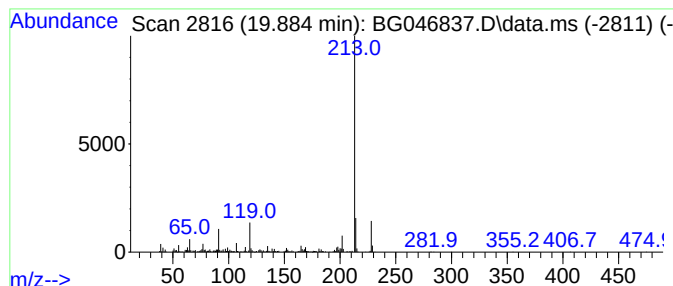
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.884	7.54 ng	448497	Chrysene-d12	21.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	91
2			2,5-bis(Trimethylsilyl)thiophene	228	C10H20SSi2	017906-71-7	45
3			2H,8H-Benzo[1,2-b:3,4-b']dipyran...	228	C14H12O3	000523-59-1	45
4			2-Trifluoromethyl-5-hydroxyquino...	213	C10H6F3NO	041958-06-9	42
5			2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	35



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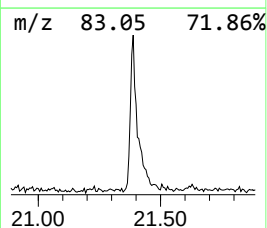
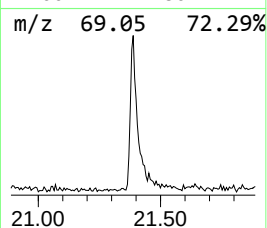
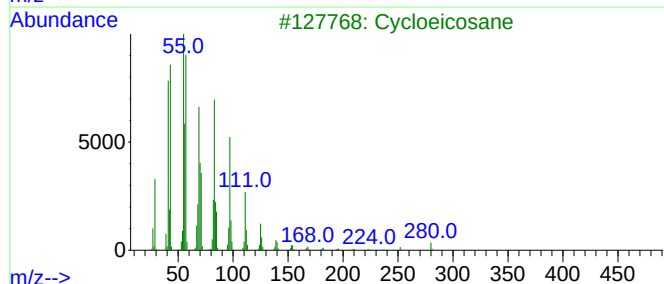
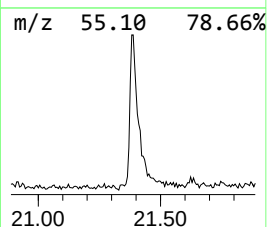
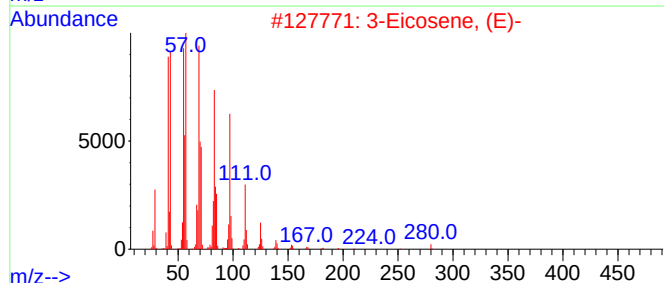
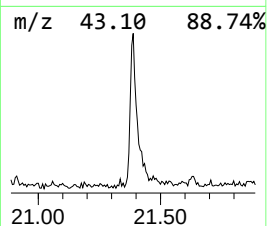
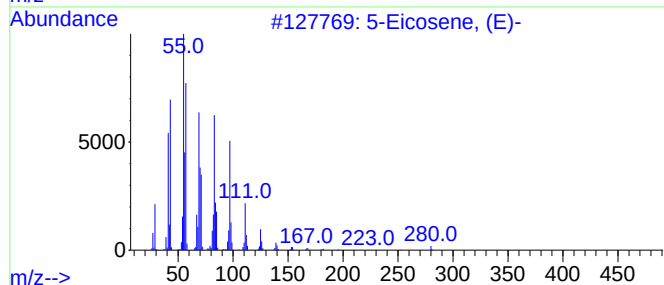
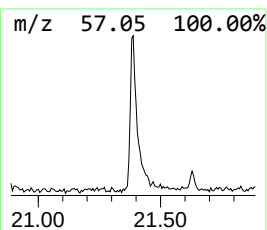
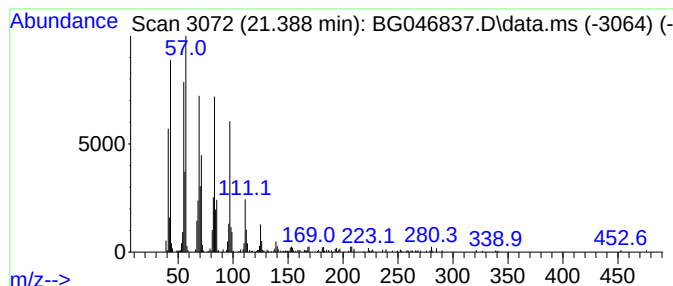
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Peak Number 4 5-Eicosene, (E)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.388	10.23 ng	608109	Chrysene-d12	21.746

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-		280	C20H40	074685-30-6	98
2	3-Eicosene, (E)-		280	C20H40	074685-33-9	97
3	Cycloeicosane		280	C20H40	000296-56-0	96
4	1-Docosene		308	C22H44	001599-67-3	95
5	1-Octadecene		252	C18H36	000112-88-9	95



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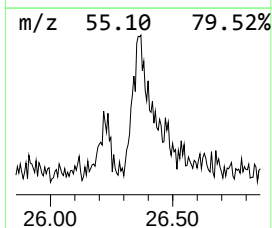
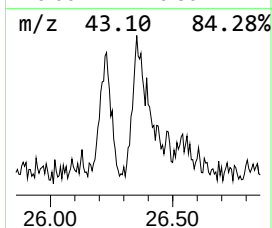
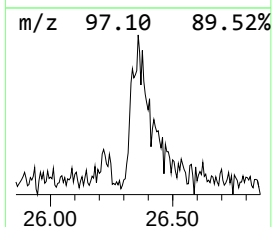
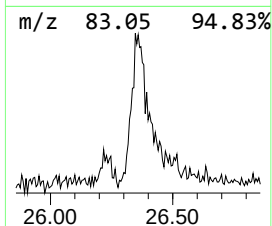
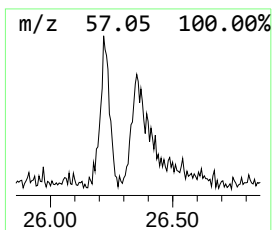
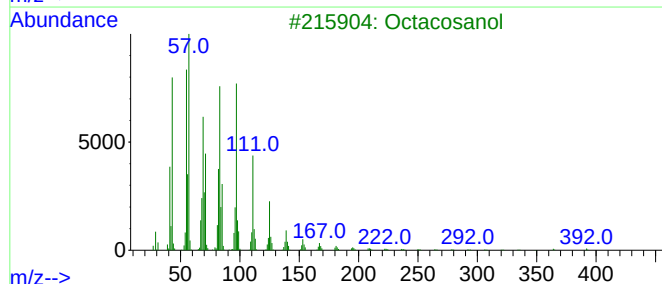
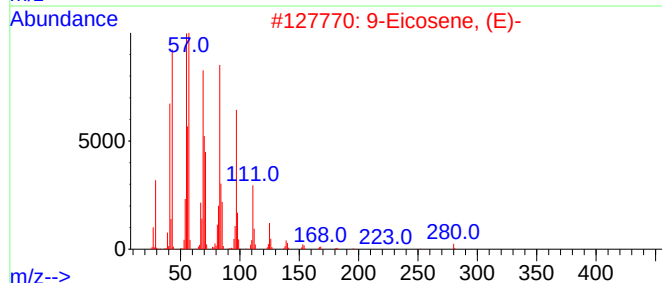
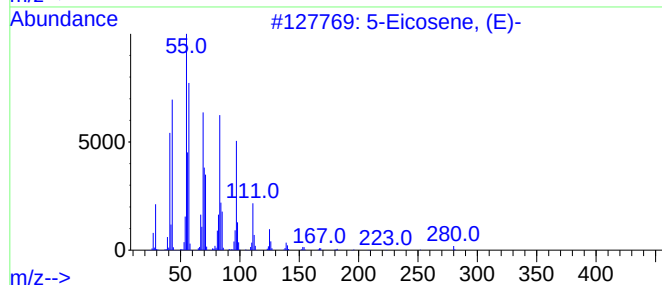
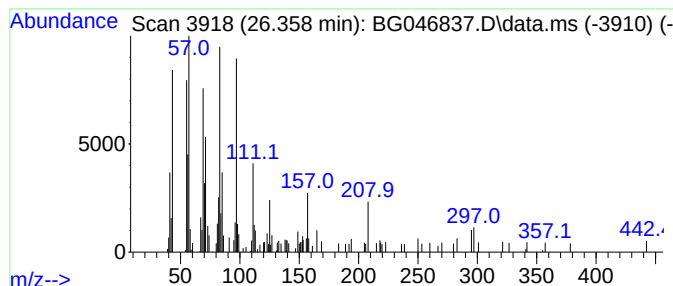
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG092220.M
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TIC Library : C:\Database\NIST11.L
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Peak Number 5 unknown26.35 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.358	3.21 ng	198817	Perylene-d12	25.007

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Eicosene, (E)-			280	C20H40	074685-30-6	70
2	9-Eicosene, (E)-			280	C20H40	074685-29-3	49
3	Octacosanol			410	C28H58O	000557-61-9	49
4	Nonadecyl trifluoroacetate			380	C21H39F3O2	1000351-76-3	49
5	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.350	7.2	ng	339486	4	17.469	946668	20.0
n-Decanoic acid	19.619	2.2	ng	130169	5	21.746	1188960	20.0
Phenol, 4,4'-(1...	19.884	7.5	ng	448497	5	21.746	1188960	20.0
5-Eicosene, (E)-	21.388	10.2	ng	608109	5	21.746	1188960	20.0
unknown26.35	26.358	3.2	ng	198817	6	25.007	1239860	20.0