

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG080323\
 Data File : BG058590.D
 Acq On : 3 Aug 2023 12:56
 Operator : MA/JU
 Sample : 03860-03
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-1A

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-BG072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG058590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.910	306	310	315	rBV	21371	31313	1.29%	0.229%
2	5.386	384	391	404	rBV	724410	1137727	46.94%	8.303%
3	6.984	656	663	677	rBV	689711	1169923	48.26%	8.538%
4	7.812	796	804	811	rBV	167329	279656	11.54%	2.041%
5	8.976	994	1002	1020	rBV	400764	716803	29.57%	5.231%
6	10.615	1273	1281	1291	rBV	217224	411667	16.98%	3.004%
7	13.077	1693	1700	1711	rBV	1053225	1632388	67.34%	11.912%
8	13.347	1741	1746	1752	rBV3	16789	27863	1.15%	0.203%
9	14.458	1928	1935	1944	rBV	365556	583526	24.07%	4.258%
10	15.950	2182	2189	2207	rBV	852331	1376318	56.78%	10.044%
11	17.201	2396	2402	2408	rBV	462676	708779	29.24%	5.172%
12	17.971	2528	2533	2542	rBV5	14203	34672	1.43%	0.253%
13	18.094	2547	2554	2565	rBV	188328	314183	12.96%	2.293%
14	19.258	2744	2752	2764	rBV	54476	106205	4.38%	0.775%
15	19.369	2767	2771	2782	rBV4	30571	58295	2.40%	0.425%
16	19.622	2810	2814	2820	rVB	42220	62372	2.57%	0.455%
17	19.822	2842	2848	2859	rBV	1806454	2424015	100.00%	17.689%
18	21.144	3068	3073	3075	rBV6	16349	32055	1.32%	0.234%
19	21.443	3117	3124	3130	rBV2	488661	823766	33.98%	6.011%
20	21.620	3151	3154	3160	rVB3	16057	24838	1.02%	0.181%
21	22.137	3237	3242	3248	rVB6	18019	30637	1.26%	0.224%
22	22.848	3360	3363	3373	rVB2	18919	30081	1.24%	0.220%
23	22.942	3374	3379	3387	rVV4	21833	51369	2.12%	0.375%
24	23.030	3387	3394	3402	rVB	114562	222430	9.18%	1.623%
25	23.183	3415	3420	3428	rVB9	17159	35832	1.48%	0.261%
26	23.535	3475	3480	3481	rBV2	20598	29059	1.20%	0.212%
27	23.606	3488	3492	3499	rVB4	38803	80222	3.31%	0.585%
28	23.911	3539	3544	3553	rVB2	27448	64919	2.68%	0.474%
29	24.223	3592	3597	3604	rVB4	16928	39652	1.64%	0.289%
30	24.364	3616	3621	3630	rVB3	13458	38651	1.59%	0.282%
31	24.516	3637	3647	3661	rBV	303322	884984	36.51%	6.458%
32	25.104	3740	3747	3758	rVB4	26059	81130	3.35%	0.592%
33	25.562	3818	3825	3833	rVB5	30768	86183	3.56%	0.629%
34	26.584	3990	3999	4010	rVB8	18708	71712	2.96%	0.523%

Sum of corrected areas: 13703225

Instrument :

BNA_G

ClientSampleId :

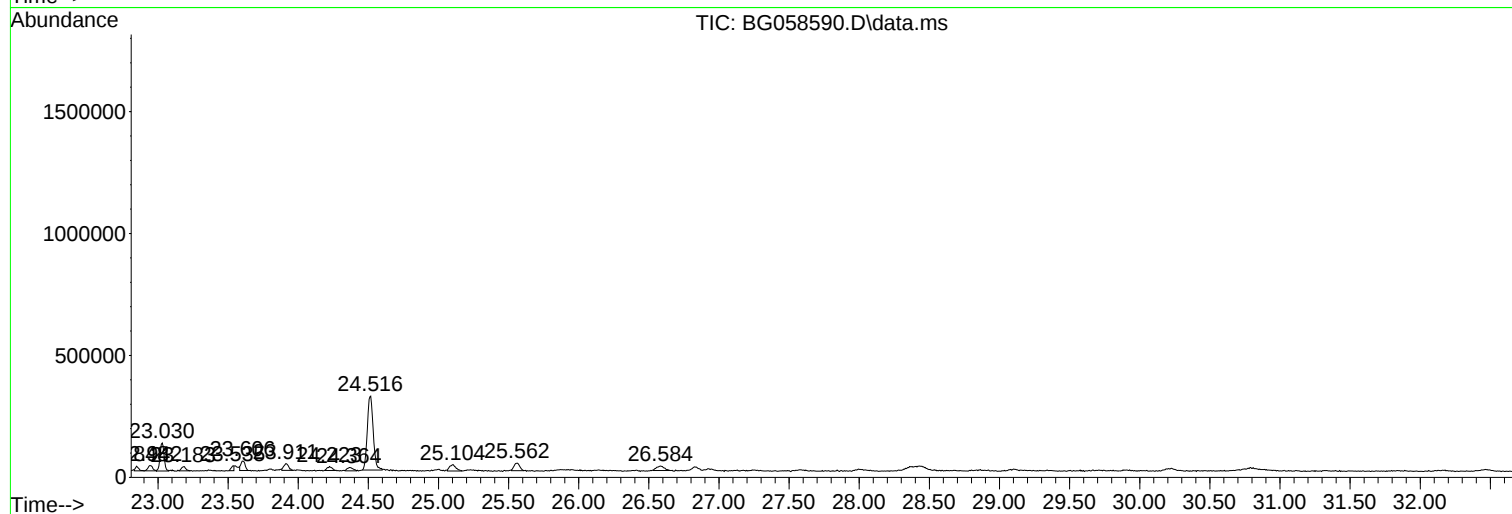
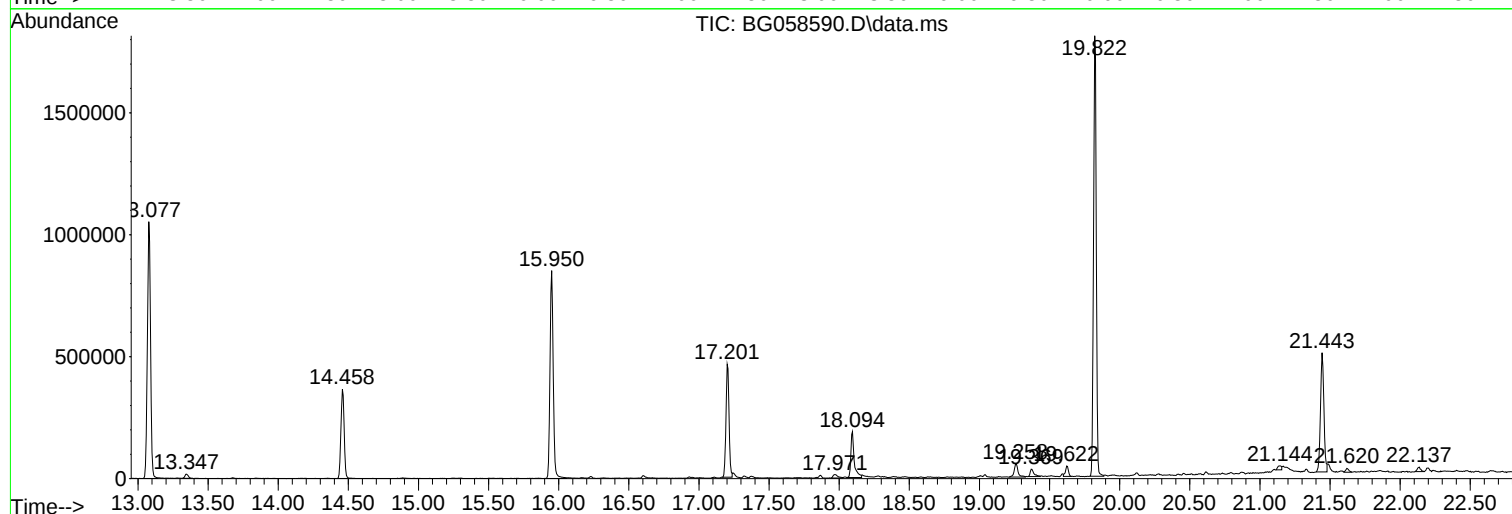
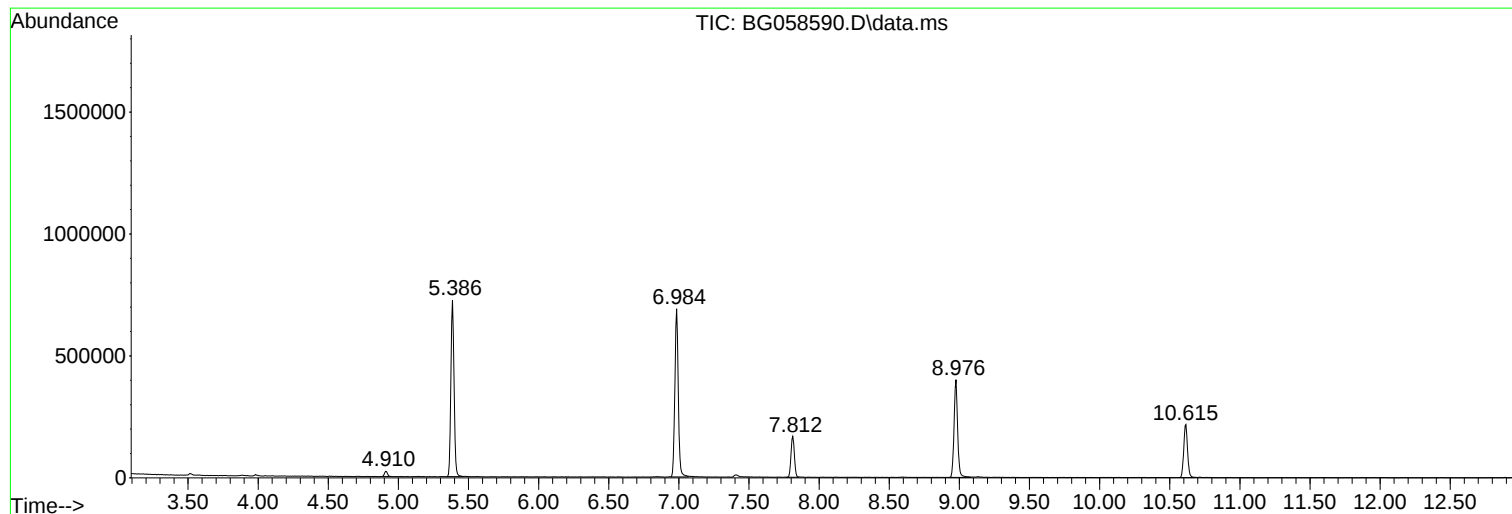
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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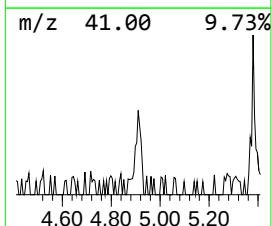
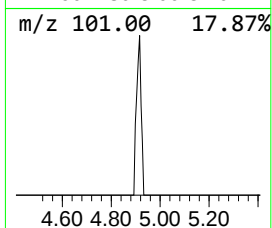
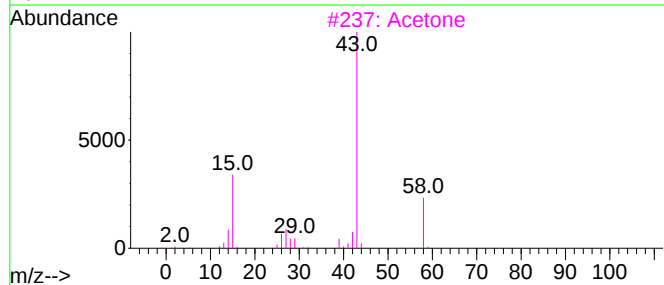
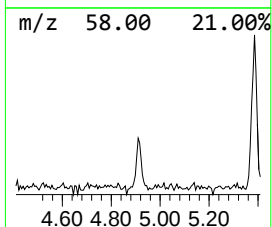
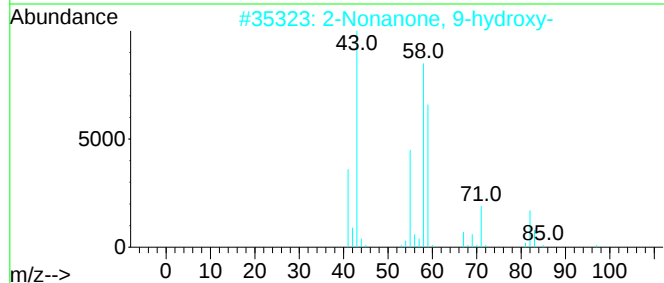
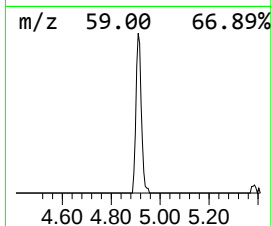
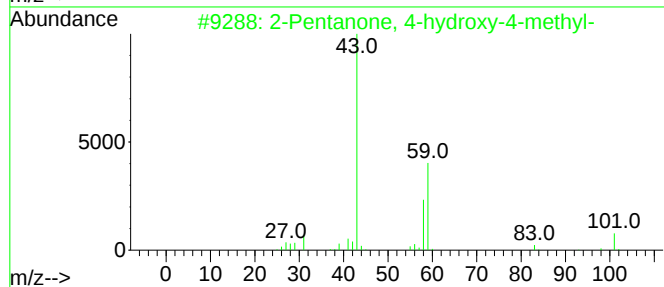
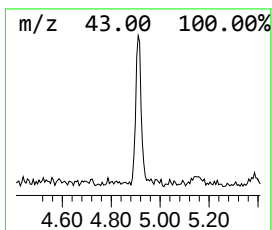
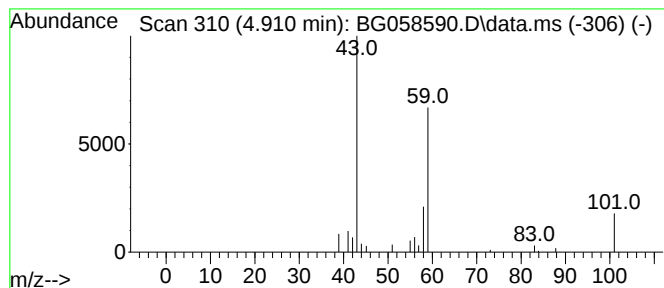
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG072823.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.910	2.24 ng	31313	1,4-Dichlorobenzene-d4	7.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	43		
2	2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	28		
3	Acetone	58	C3H6O	000067-64-1	9		
4	1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9		
5	3-Hexanol	102	C6H14O	000623-37-0	9		



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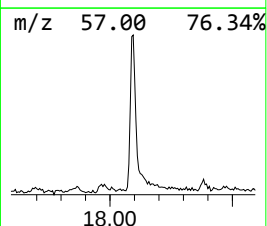
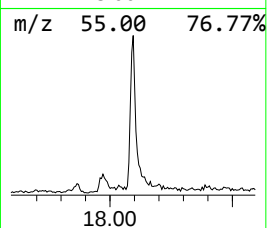
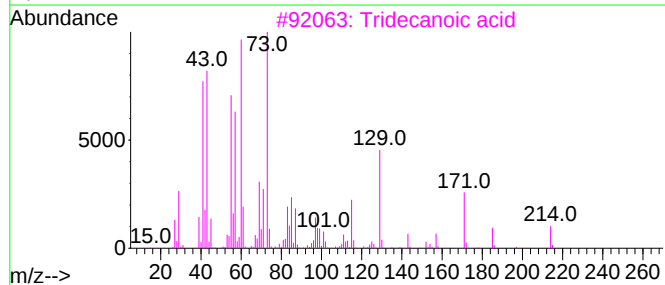
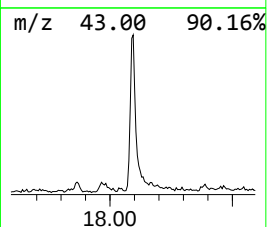
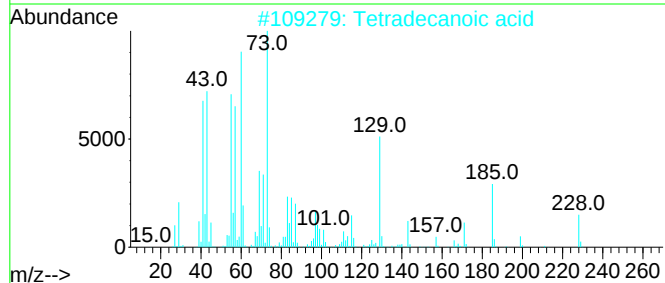
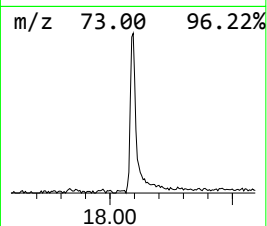
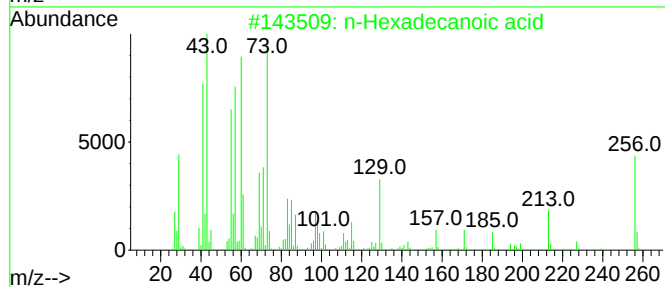
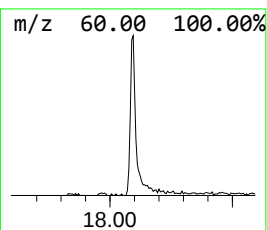
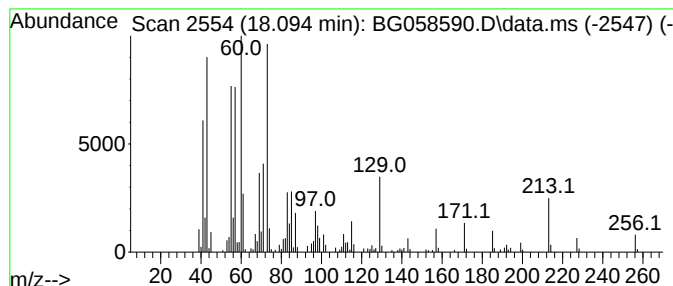
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.094	8.87 ng	314183	Phenanthrene-d10	17.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	90
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Undecanoic acid	186	C11H22O2	000112-37-8	74



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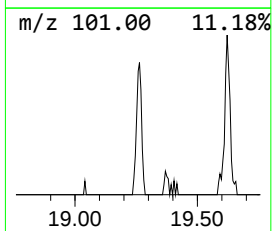
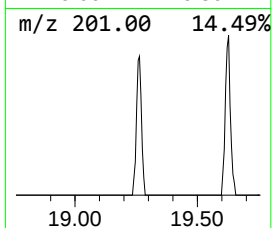
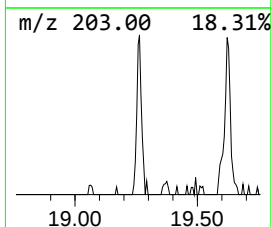
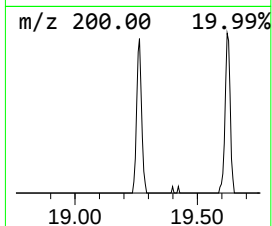
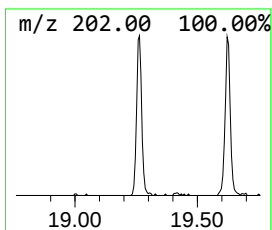
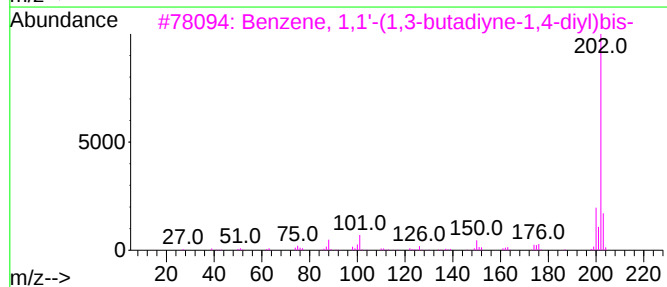
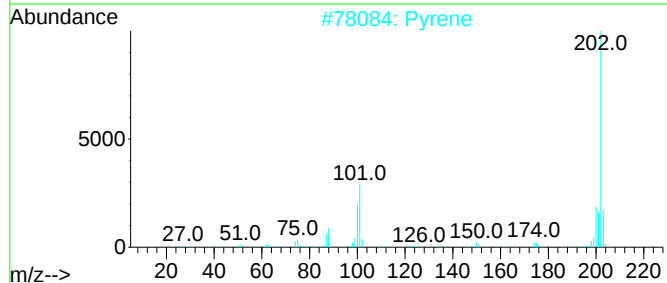
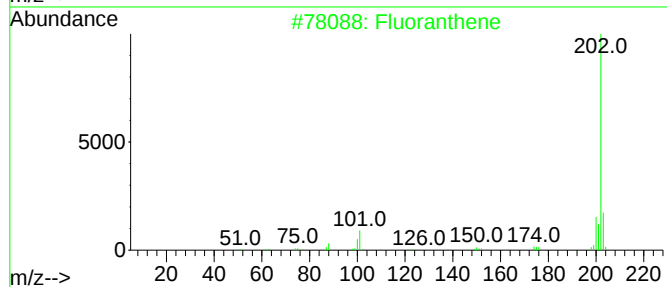
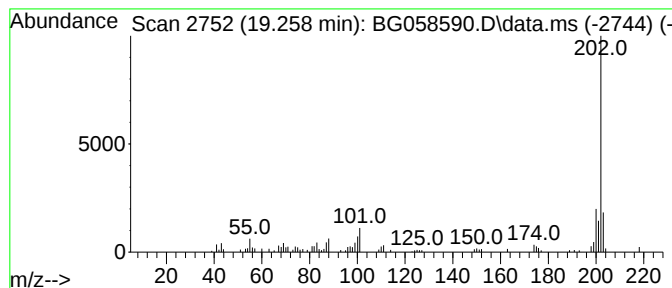
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Peak Number 3 Benzene, 1,1'-(1,3-butadiyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.258	3.00 ng	106205	Phenanthrene-d10	17.201

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fluoranthene	202	C16H10	000206-44-0	94
2			Pyrene	202	C16H10	000129-00-0	89
3			Benzene, 1,1'-(1,3-butadiyne-1,4...	202	C16H10	000886-66-8	76
4			4-Benzyl-1-(1-methyl-2-[(trimeth...	469	C27H43NO2Si2	1000408-11-0	38
5			7H-Furo[3,2-g][1]benzopyran-7-on...	202	C11H6O4	002009-24-7	38



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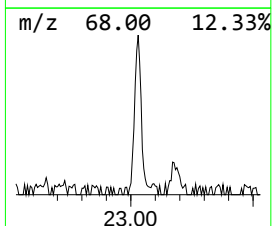
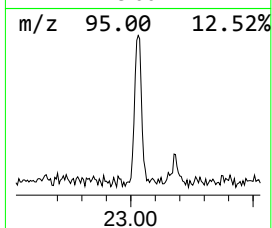
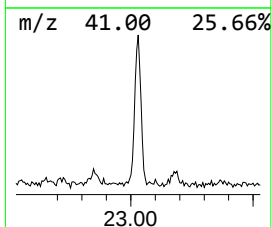
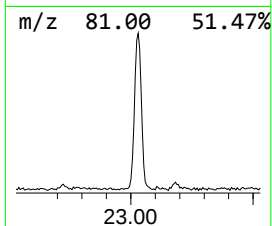
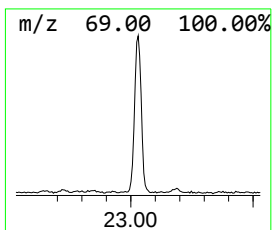
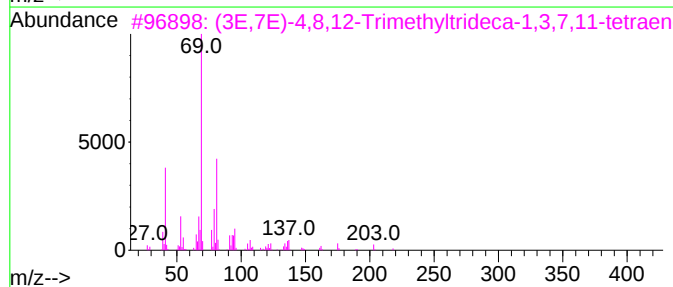
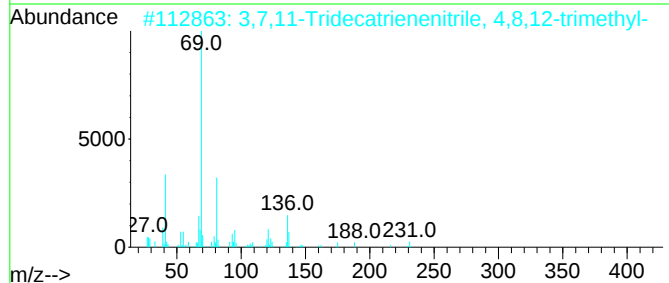
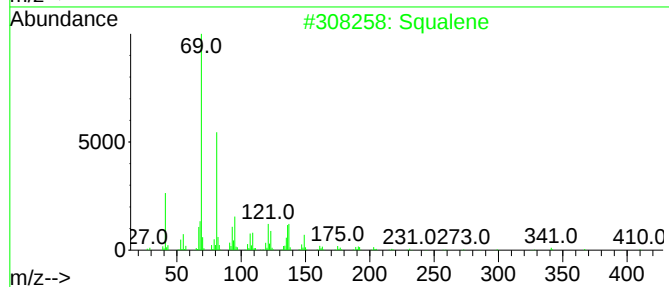
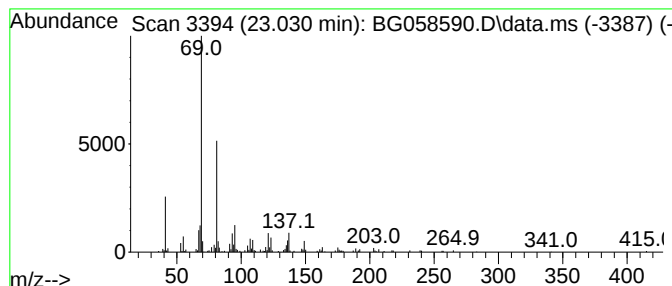
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Peak Number 4 Squalene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.030	5.03 ng	222430	Perylene-d12	24.516

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	90
2			3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	72
3			(3E,7E)-4,8,12-Trimethyltrideca...	218	C16H26	062235-06-7	72
4			1,5,9-Decatriene, 2,3,5,8-tetram...	192	C14H24	230646-72-7	72
5			3,7-Dimethyl-1-phenylsulfonyl-2,...	278	C16H22O2S	1000432-27-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.910	2.2	ng	31313	1	7.812	279656	20.0
n-Hexadecanoic ...	18.094	8.9	ng	314183	4	17.201	708779	20.0
Benzene, 1,1'-(...	19.258	3.0	ng	106205	4	17.201	708779	20.0
Squalene	23.030	5.0	ng	222430	6	24.516	884984	20.0