

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG042321\
 Data File : BG048867.D
 Acq On : 23 Apr 2021 17:31
 Operator : CG/JU
 Sample : M2107-17
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-34-0-2.0

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-BG041421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG048867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.611	379	387	396	rBV	420793	686598	58.59%	9.126%
2	7.221	653	661	670	rBV	449828	771777	65.86%	10.259%
3	8.055	796	803	810	rBV	111527	183310	15.64%	2.437%
4	9.230	993	1003	1014	rBV	296191	515137	43.96%	6.847%
5	10.881	1278	1284	1291	rVB	145635	250077	21.34%	3.324%
6	13.331	1694	1701	1708	rBV	670673	995783	84.97%	13.236%
7	14.154	1834	1841	1849	rBV	20193	32776	2.80%	0.436%
8	14.712	1928	1936	1943	rBV2	211778	355360	30.32%	4.724%
9	16.210	2183	2191	2200	rBV	516043	780209	66.58%	10.371%
10	17.473	2397	2406	2411	rBV	253448	393132	33.55%	5.226%
11	18.361	2551	2557	2561	rBV5	10901	18666	1.59%	0.248%
12	19.459	2739	2744	2749	rBV5	23323	33136	2.83%	0.440%
13	19.524	2751	2755	2760	rBV	21808	31856	2.72%	0.423%
14	19.888	2813	2817	2822	rVV	24790	36575	3.12%	0.486%
15	20.082	2844	2850	2857	rBV	903990	1171897	100.00%	15.577%
16	20.764	2962	2966	2970	rVB7	8331	12588	1.07%	0.167%
17	20.869	2980	2984	2987	rVB6	11225	13218	1.13%	0.176%
18	21.381	3067	3071	3081	rBV3	103833	153781	13.12%	2.044%
19	21.768	3130	3137	3143	rBV2	222466	388925	33.19%	5.170%
20	21.815	3143	3145	3149	rVB4	12439	14182	1.21%	0.189%
21	22.597	3269	3278	3283	rBV4	41953	104144	8.89%	1.384%
22	24.113	3532	3536	3542	rVB6	29560	56585	4.83%	0.752%
23	24.771	3643	3648	3652	rBV8	11249	22831	1.95%	0.303%
24	25.094	3694	3703	3715	rVB	138212	392295	33.48%	5.215%
25	25.799	3821	3823	3826	rBV4	9096	11977	1.02%	0.159%
26	26.269	3895	3903	3917	rVB10	29624	96330	8.22%	1.280%

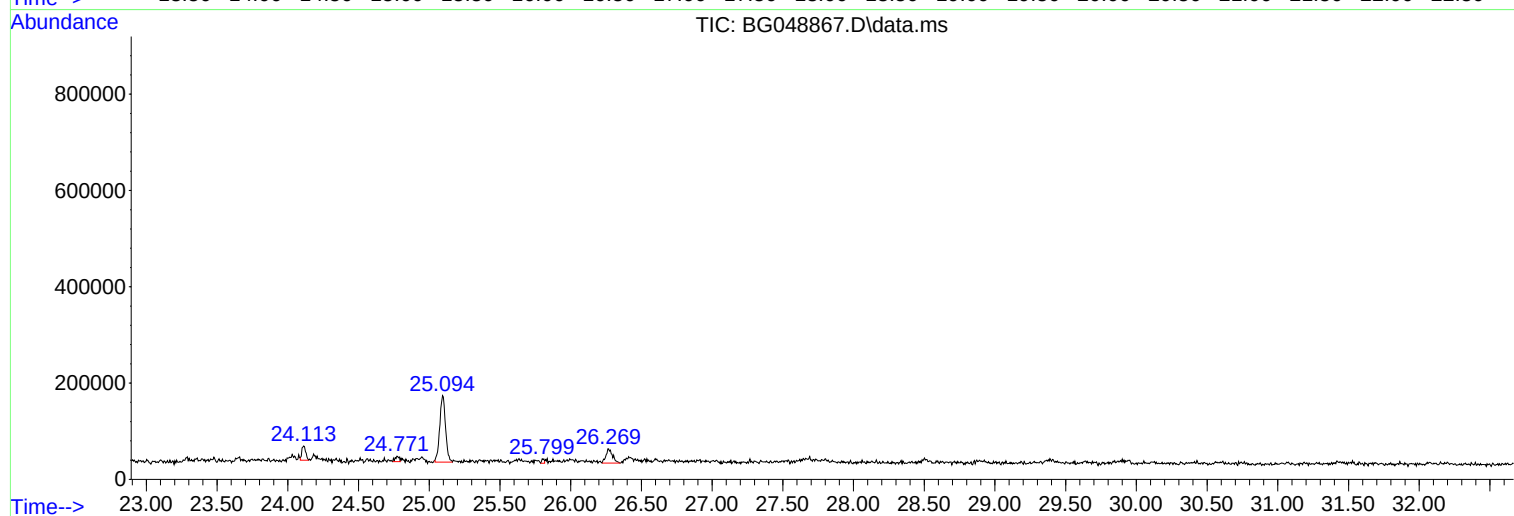
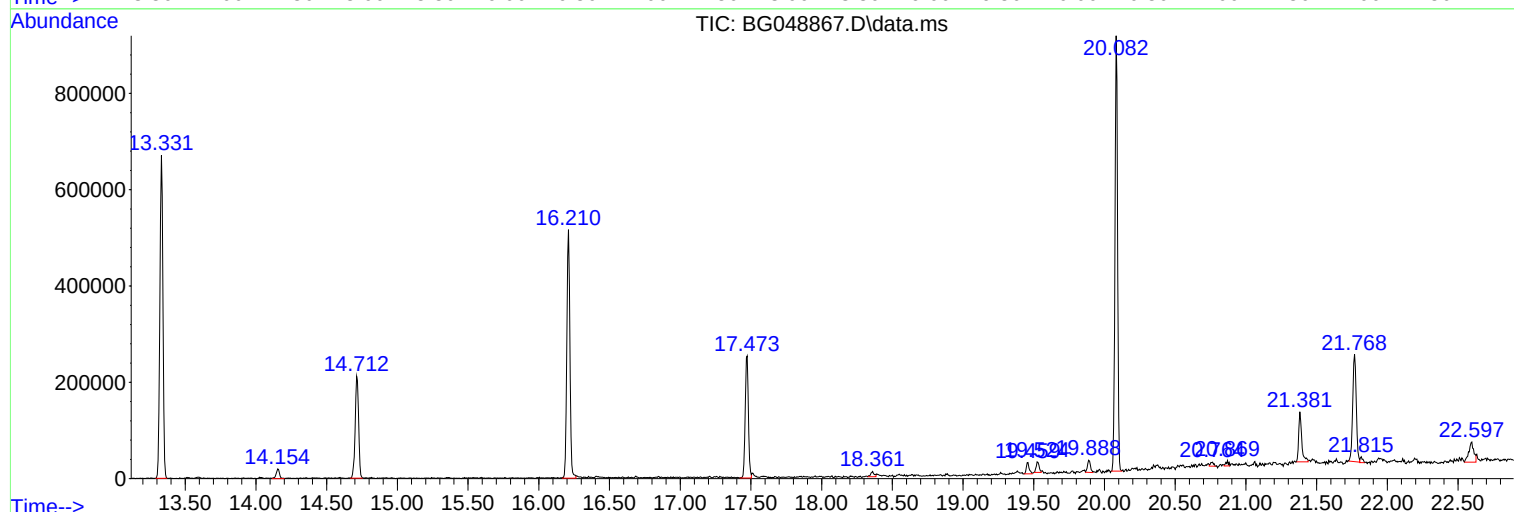
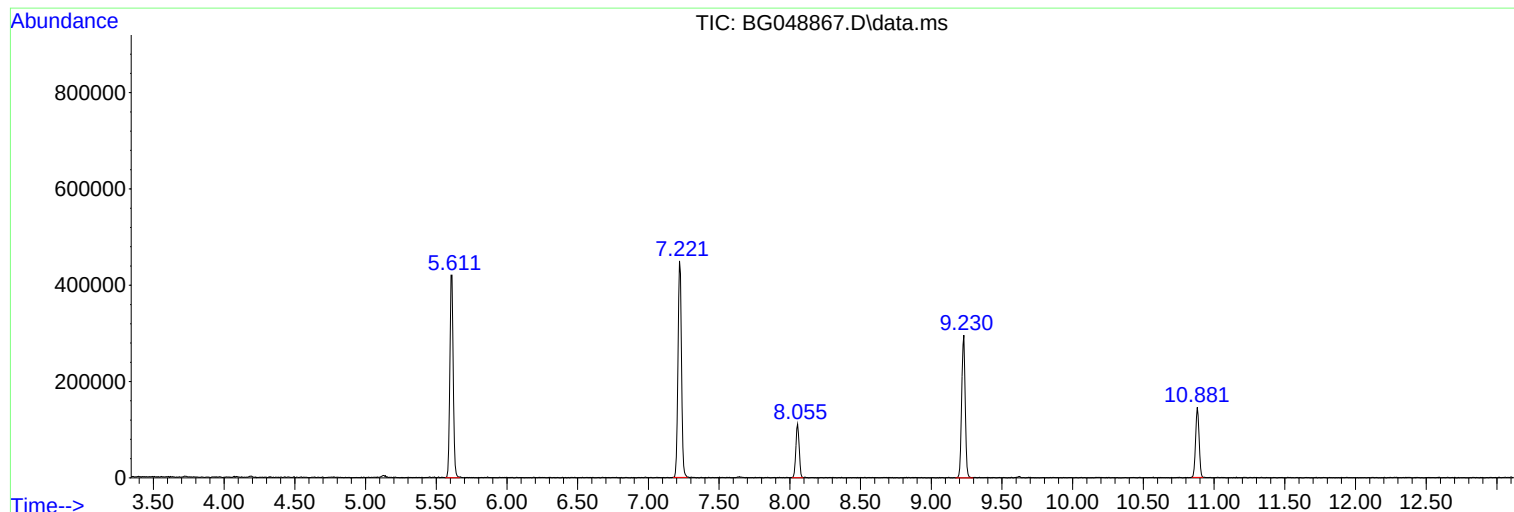
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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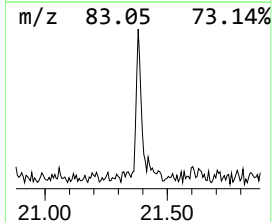
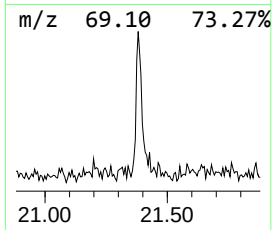
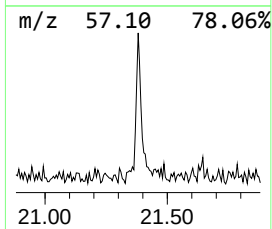
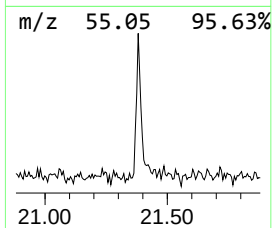
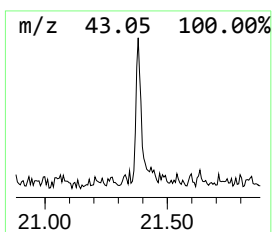
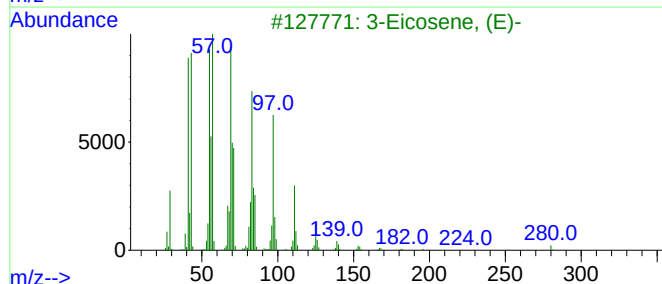
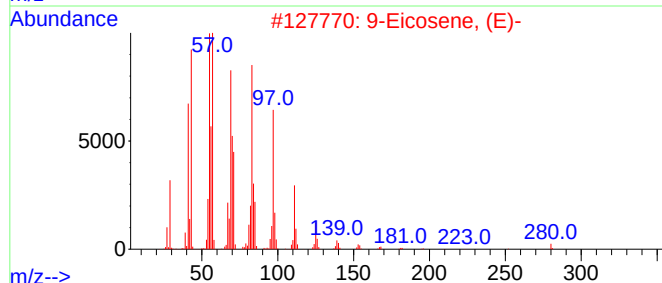
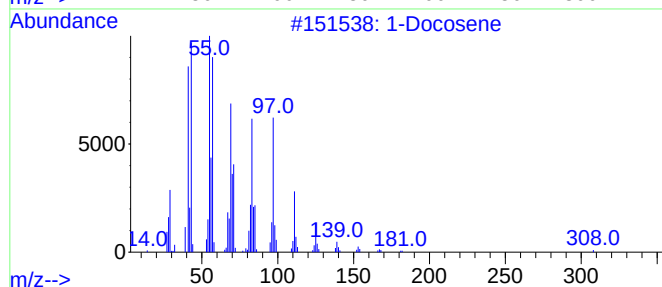
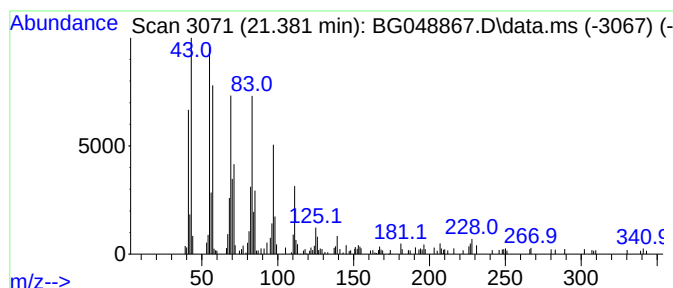
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.381	7.91 ng	153781	Chrysene-d12	21.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	93
2	9-Eicosene, (E)-			280	C20H40	074685-29-3	93
3	3-Eicosene, (E)-			280	C20H40	074685-33-9	93
4	n-Tetracosanol-1			354	C24H50O	000506-51-4	91
5	Cyclodocosane, ethyl-			336	C24H48	1000151-22-6	90



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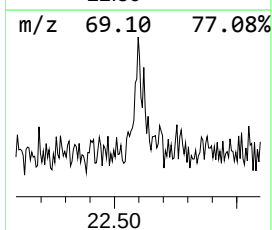
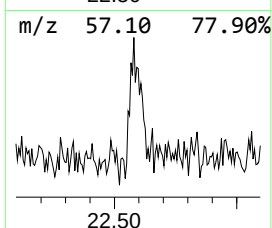
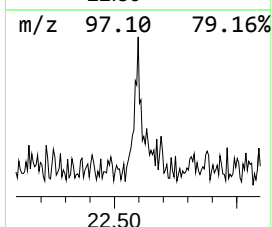
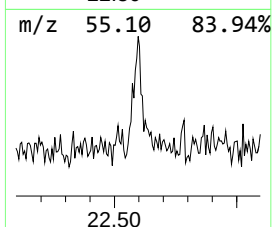
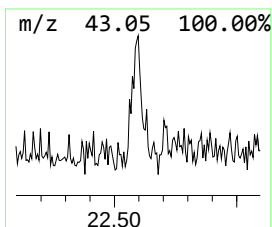
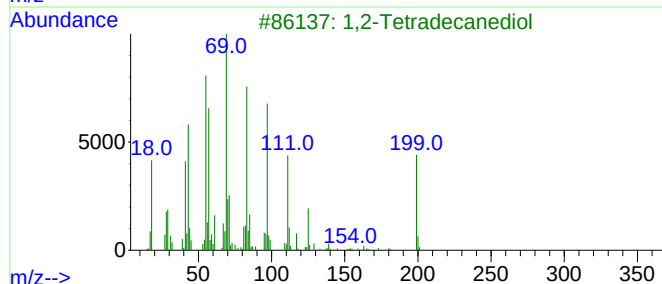
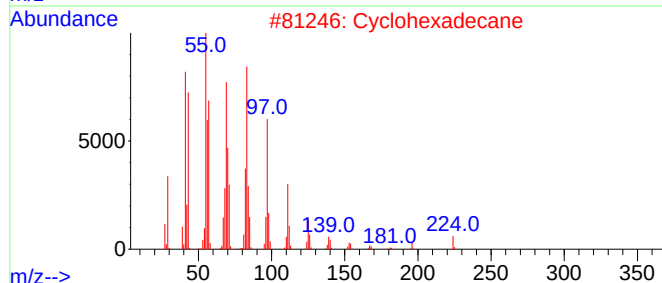
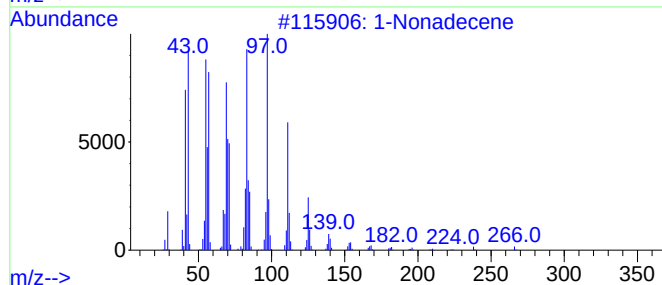
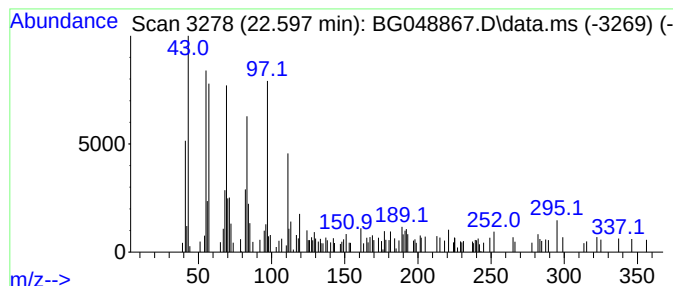
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG041421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 1-Nonadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.597	5.36 ng	104144	Chrysene-d12	21.768

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	83
2	Cyclohexadecane			224	C16H32	000295-65-8	58
3	1,2-Tetradecanediol			230	C14H30O2	021129-09-9	52
4	4-n-Hexylthiane, S,S-dioxide			218	C11H22O2S	070928-52-8	50
5	7-Hexadecene, (Z)-			224	C16H32	035507-09-6	46



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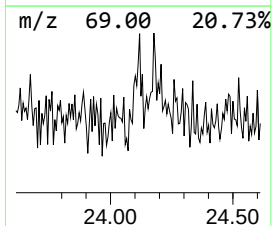
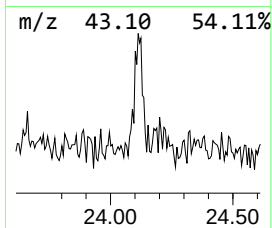
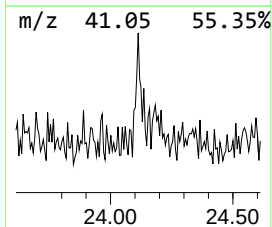
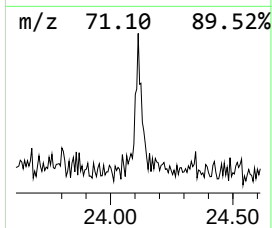
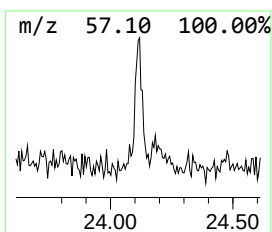
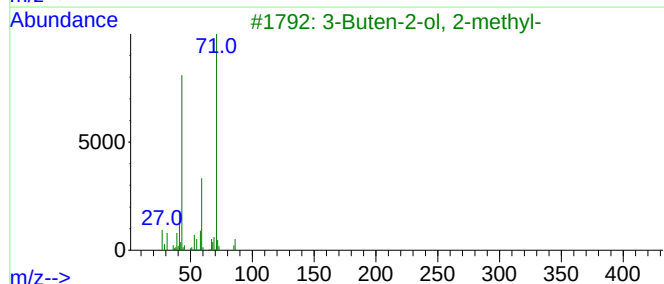
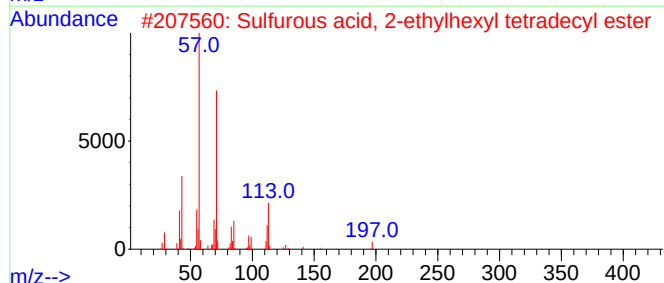
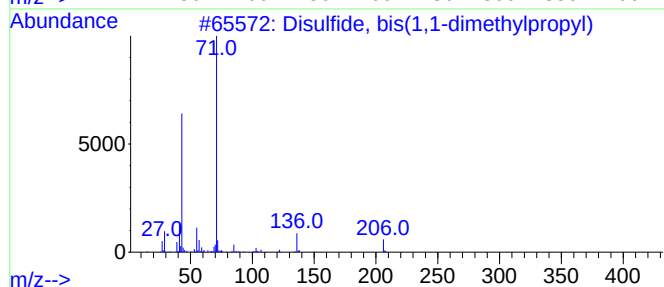
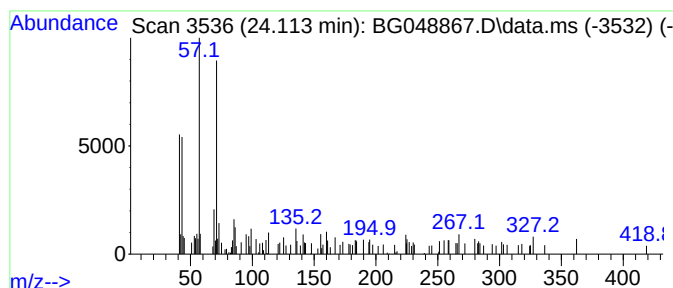
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Peak Number 3 unknown24.11 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.113	2.88 ng	56585	Perylene-d12	25.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Disulfide, bis(1,1-dimethylpropyl)	206	C10H22S2	034965-30-5	49
2			Sulfurous acid, 2-ethylhexyl tet...	390	C22H46O3S	1000309-19-7	49
3			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	49
4			trans-1-Methoxy-1-butene	86	C5H10O	010034-13-6	49
5			3-Heptanone, 2,4-dimethyl-	142	C9H18O	018641-71-9	49



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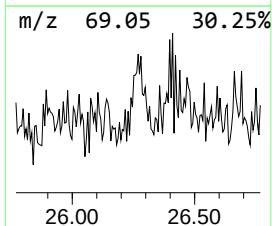
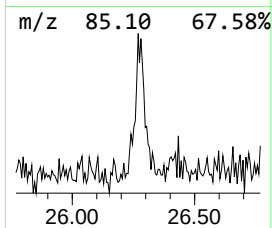
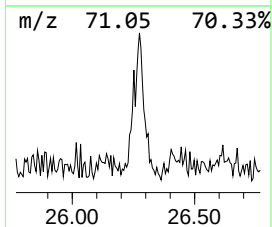
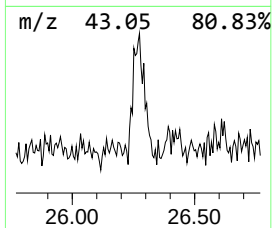
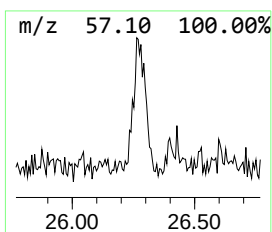
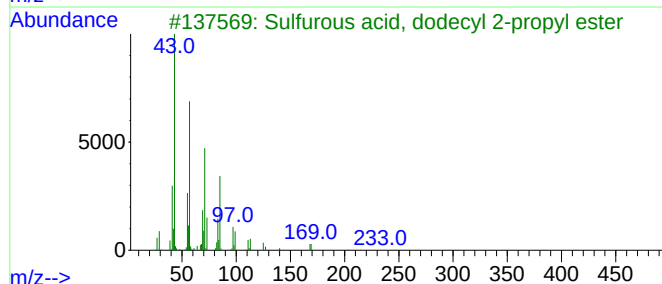
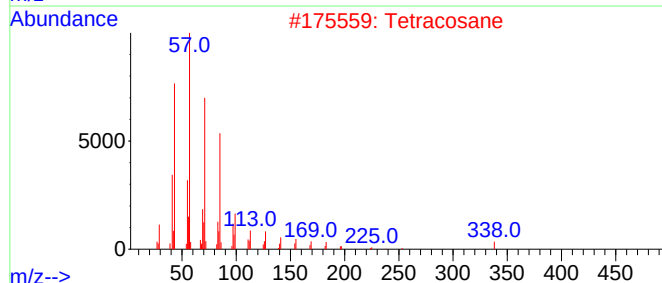
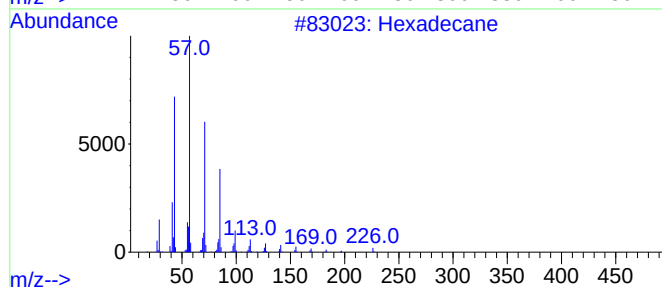
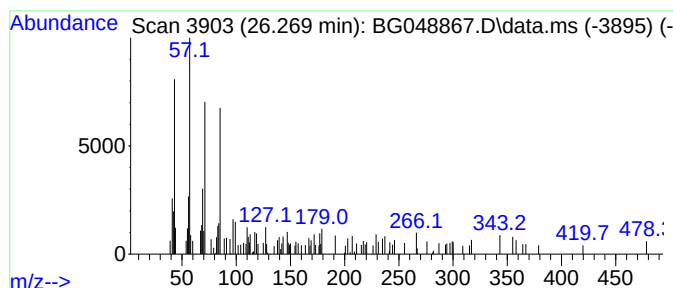
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Peak Number 4 Hexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.269	4.91 ng	96330	Perylene-d12	25.094

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecane	226	C16H34	000544-76-3	60
2			Tetracosane	338	C24H50	000646-31-1	49
3			Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	49
4			Eicosane	282	C20H42	000112-95-8	49
5			Sulfurous acid, butyl tetradecyl...	334	C18H38O3S	1000309-18-1	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Docosene	21.381	7.9	ng	153781	5	21.768	388925	20.0
1-Nonadecene	22.597	5.4	ng	104144	5	21.768	388925	20.0
unknown24.11	24.113	2.9	ng	56585	6	25.094	392295	20.0
Hexadecane	26.269	4.9	ng	96330	6	25.094	392295	20.0