

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM082718\
 Data File : BM016626.D
 Acq On : 28 Aug 2018 04:03
 Operator : SJ/JU
 Sample : J4660-14
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 082318-TIPC-F-D-S

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082118.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.546	380	384	399	rBV	378429	743904	3.69%	1.385%
2	7.181	658	662	672	rBV	218452	437252	2.17%	0.814%
3	7.528	713	721	738	rBV	1095614	1922483	9.54%	3.580%
4	8.004	796	802	817	rBV2	333444	644638	3.20%	1.200%
5	8.316	848	855	869	rBV	2067516	3334466	16.55%	6.210%
6	9.187	995	1003	1019	rBV	1184381	2066108	10.25%	3.848%
7	10.810	1272	1279	1297	rBV	372216	730320	3.62%	1.360%
8	13.257	1683	1695	1710	rBV	5681408	7538786	37.42%	14.039%
9	14.645	1923	1931	1945	rBV2	666570	1109013	5.50%	2.065%
10	16.133	2178	2184	2199	rBV	3510277	5269796	26.15%	9.814%
11	17.386	2391	2397	2411	rBV	1199315	1713823	8.51%	3.192%
12	18.239	2537	2542	2549	rBV2	350131	494795	2.46%	0.921%
13	19.974	2831	2837	2849	rBV	18419941	20148816	100.00%	37.522%
14	21.204	3043	3046	3052	rBV6	110868	206445	1.02%	0.384%
15	21.527	3097	3101	3111	rBV	1978666	2774109	13.77%	5.166%
16	22.515	3265	3269	3279	rVB	905371	1363991	6.77%	2.540%
17	22.651	3289	3292	3297	rVB	266032	345951	1.72%	0.644%
18	23.809	3483	3489	3498	rBV2	1392116	2854568	14.17%	5.316%

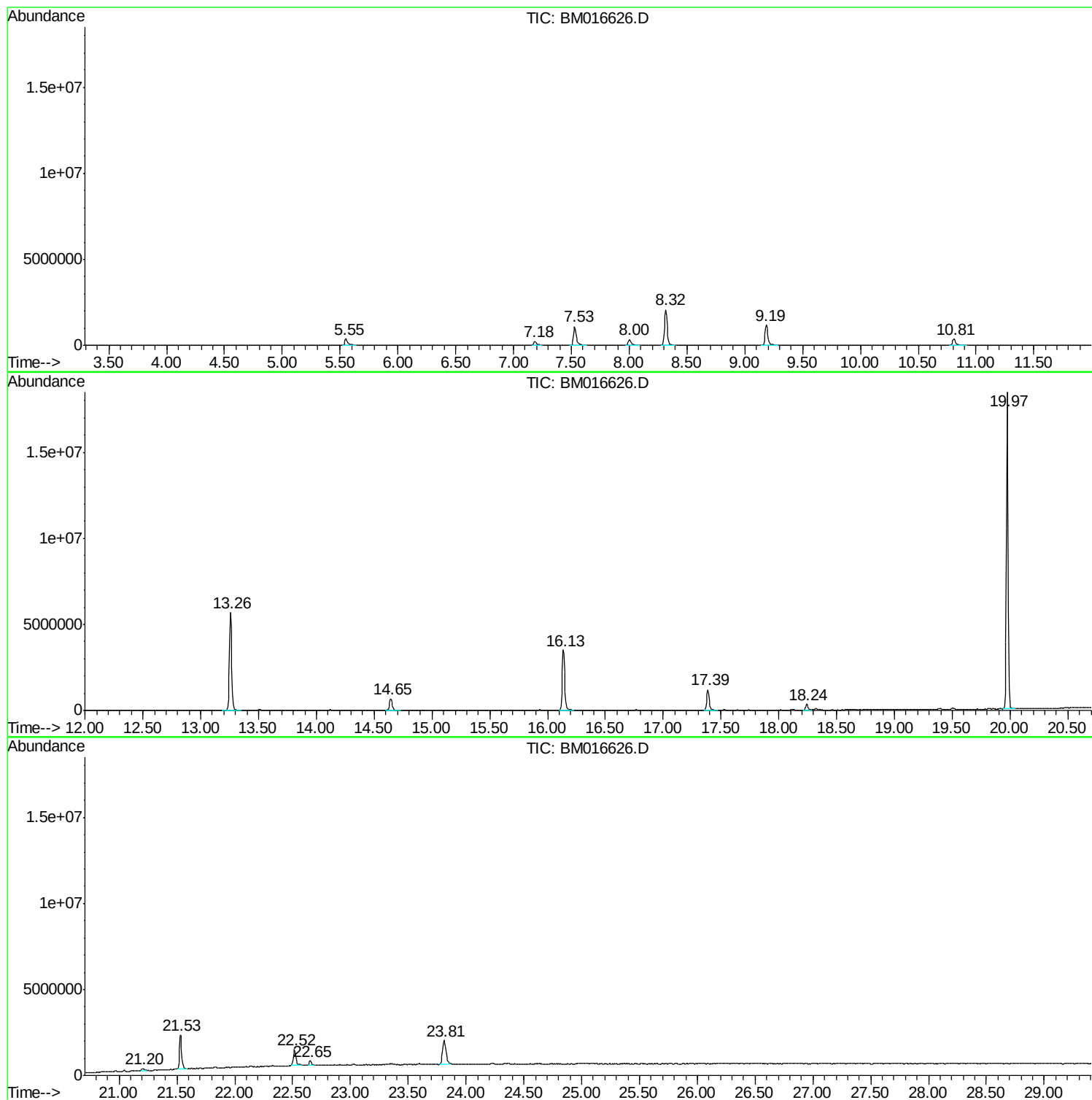
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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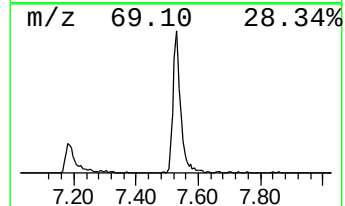
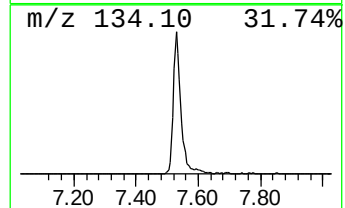
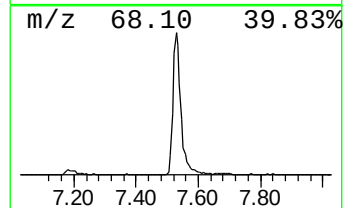
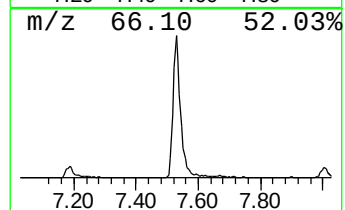
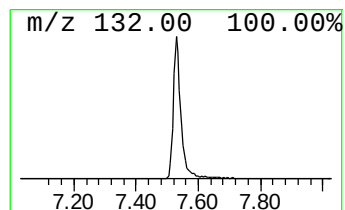
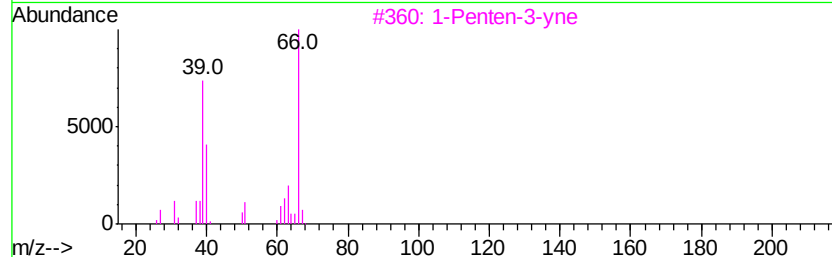
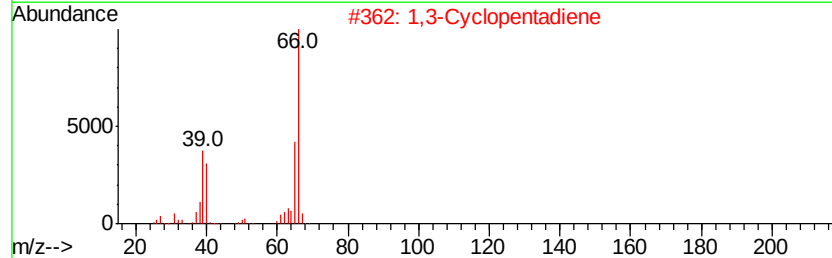
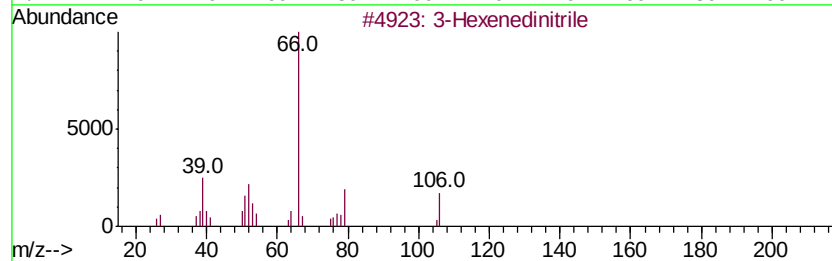
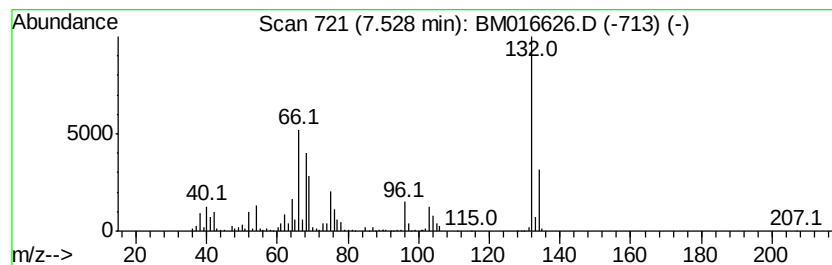
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.53 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	59.65 ng	1922480	1,4-Dichlorobenzene-d4	8.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Hexenedinitrile	106	C6H6N2	001119-85-3	25
2		1,3-Cyclopentadiene	66	C5H6	000542-92-7	25
3		1-Penten-3-yne	66	C5H6	000646-05-9	25
4		1,4,4a,8a-Tetrahydro-1,4-methano...	174	C11H10O2	001200-89-1	25
5		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14



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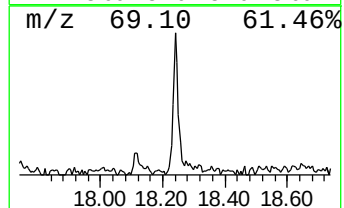
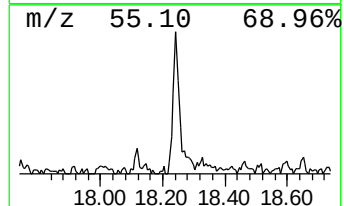
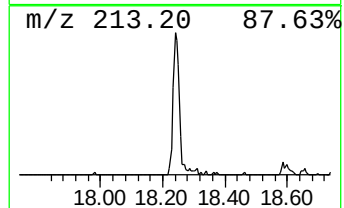
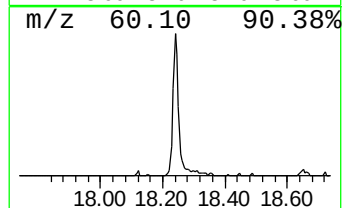
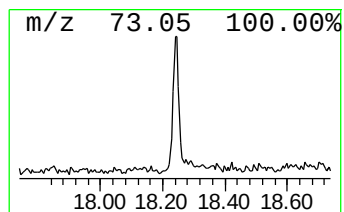
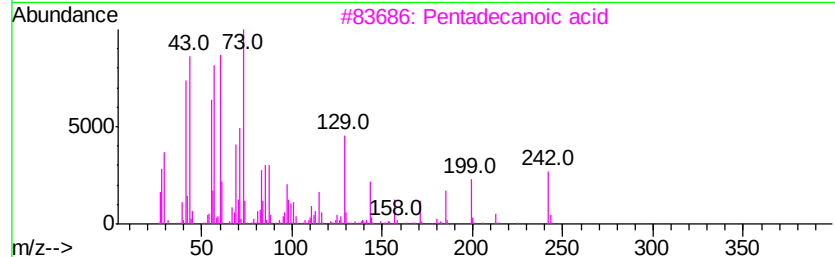
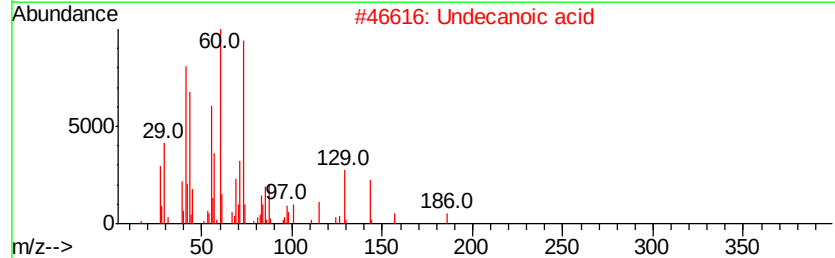
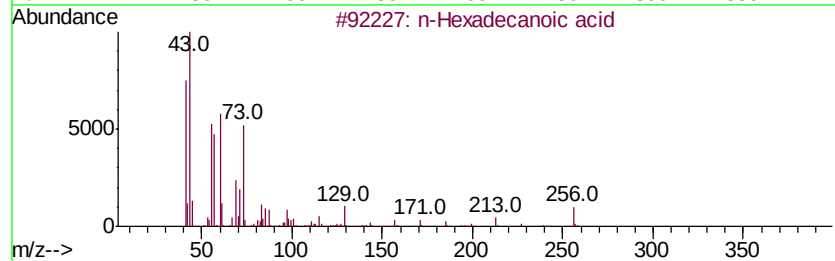
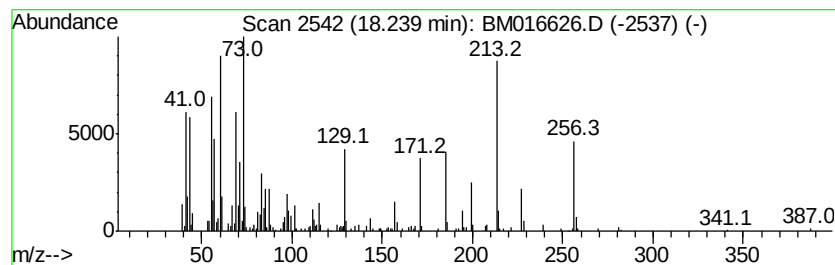
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.
18.24	5.77 ng	494795	Phenanthrene-d10		17.39
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2	Undecanoic acid	186	C11H22O2	000112-37-8	44
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	42
4	n-Decanoic acid	172	C10H20O2	000334-48-5	35
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	30



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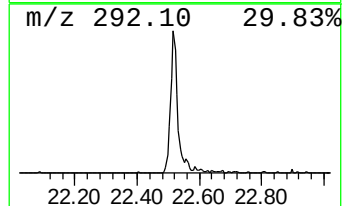
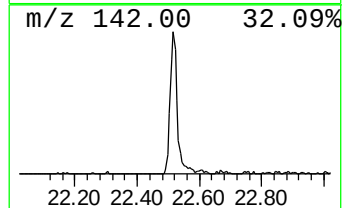
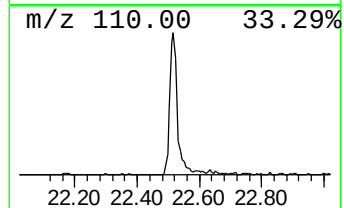
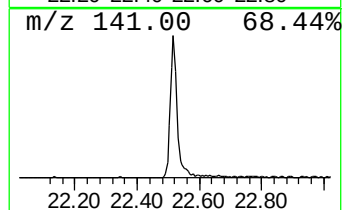
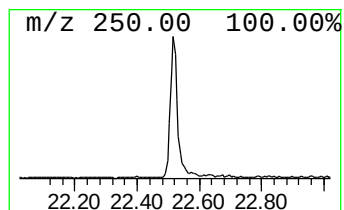
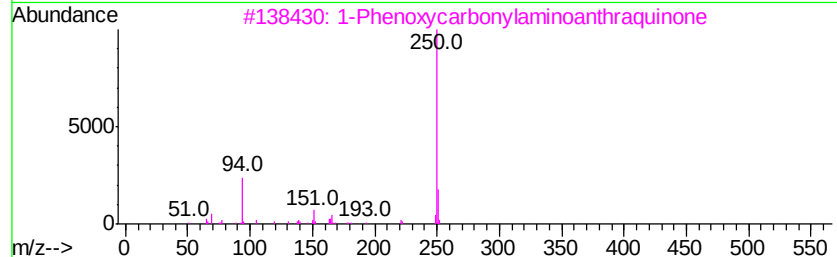
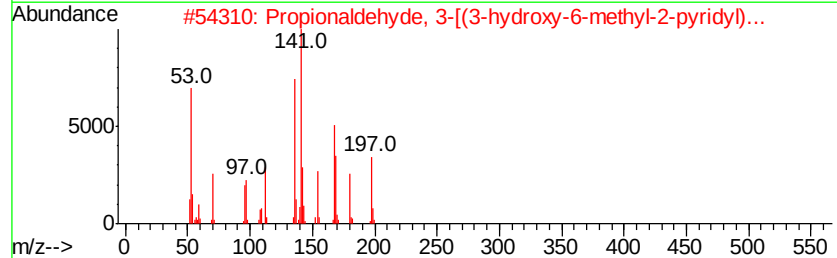
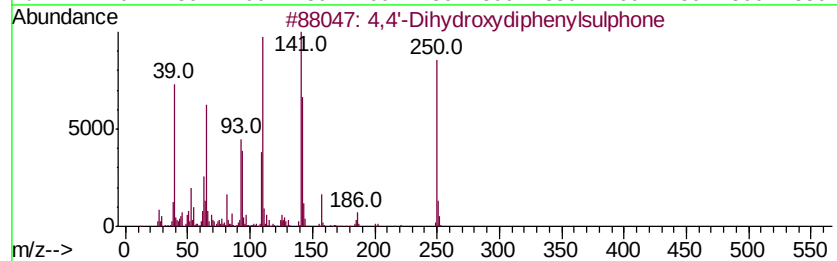
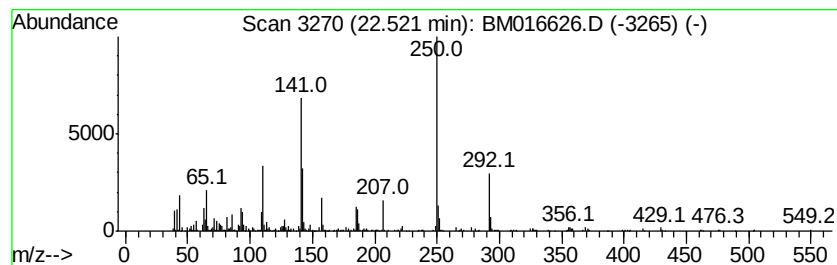
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Peak Number 4 4,4'-Dihydroxydiphenylsulphone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
22.52	9.83 ng	1363990	Chrysene-d12	21.53	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,4'-Dihydroxydiphenylsulphone	250	C12H10O4S	000080-09-1	86
2	Propionaldehyde, 3-[(3-hydroxy-6-methyl-2-pyridyl)]...	197	C9H11NO2S	030221-77-3	27
3	1-Phenoxy-carbonylaminoanthraquinone	343	C21H13N04	092506-12-2	22
4	2,6-Difluorobenzoic acid, pent-2-yl ester	222	C12H8F2O2	1000292-58-3	22
5	dl-p-Chloro-alpha-hydroxyphenylalanine	186	C8H7ClO3	007138-34-3	22



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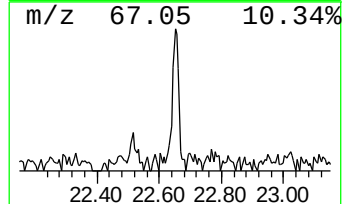
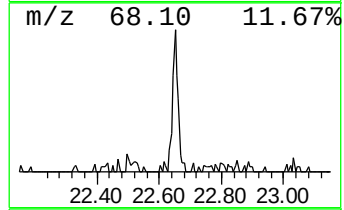
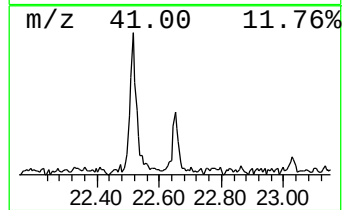
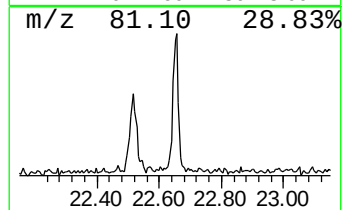
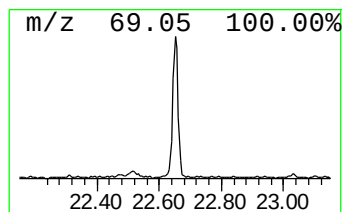
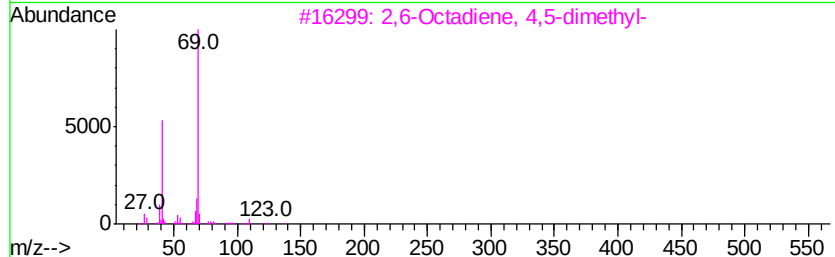
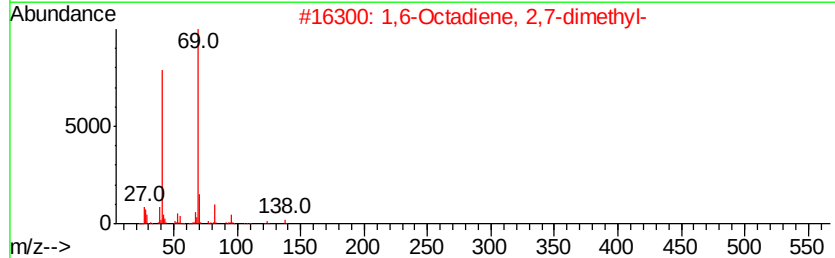
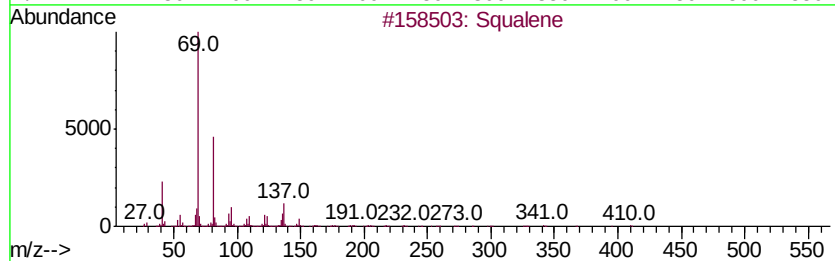
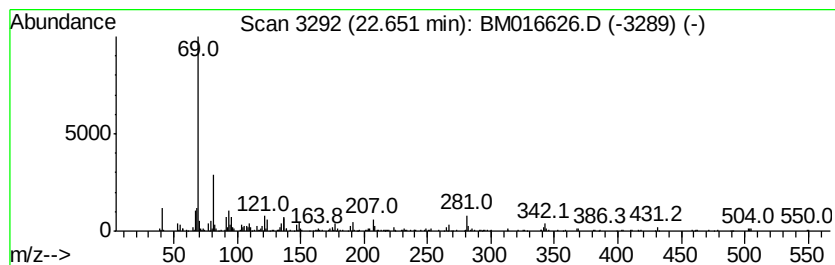
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.65	2.49 ng	345951	Chrysene-d12	21.53

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	68
2		1,6-Octadiene, 2,7-dimethyl-	138	C10H18	040195-09-3	64
3		2,6-Octadiene, 4,5-dimethyl-	138	C10H18	018476-57-8	59
4		2,6-Octadien-1-ol, 3,7-dimethyl-...	182	C11H18O2	000105-86-2	59
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.53	7.53	59.6	ng	1922480	1	8.00	644638	20.0
n-Hexadecanoic acid	18.24	5.8	ng	494795	4	17.39	1713820	20.0
4,4'-Dihydroxydip...	22.52	9.8	ng	1363990	5	21.53	2774110	20.0
Squalene	22.65	2.5	ng	345951	5	21.53	2774110	20.0