

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM022719\
 Data File : BM018953.D
 Acq On : 27 Feb 2019 17:21
 Operator : JU/SJ
 Sample : K1627-04
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 SB-02-(5-10)

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_M\METHODS\8270-BM021119.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	5.287	367	374	393	rBV	3677562	5702748	55.25%	7.487%
2	6.869	635	643	665	rBV	4081456	6615580	64.10%	8.685%
3	7.228	696	704	718	rBV	4063988	6576554	63.72%	8.634%
4	7.693	776	783	790	rBV	848887	1364186	13.22%	1.791%
5	8.004	825	836	848	rBV	2650953	4300272	41.66%	5.646%
6	8.857	974	981	998	rBV	2285487	3927360	38.05%	5.156%
7	10.481	1250	1257	1272	rBV	1166553	2032617	19.69%	2.668%
8	12.957	1670	1678	1692	rBV	5088779	7351153	71.22%	9.651%
9	13.804	1815	1822	1835	rBV	344227	536028	5.19%	0.704%
10	14.339	1907	1913	1929	rVB2	1779408	2826425	27.38%	3.711%
11	15.839	2162	2168	2187	rBV	5534887	7624318	73.87%	10.009%
12	17.098	2376	2382	2387	rBV2	2323109	3381569	32.76%	4.439%
13	17.857	2505	2511	2518	rBV2	113868	185935	1.80%	0.244%
14	17.986	2527	2533	2544	rBV	817436	1249716	12.11%	1.641%
15	19.145	2724	2730	2737	rBV3	75427	179357	1.74%	0.235%
16	19.268	2747	2751	2759	rBV2	178103	273517	2.65%	0.359%
17	19.409	2771	2775	2781	rBV	431758	481516	4.67%	0.632%
18	19.727	2824	2829	2835	rBV	8427862	10321521	100.00%	13.550%
19	20.992	3040	3044	3052	rBV	439241	600631	5.82%	0.789%
20	21.292	3090	3095	3100	rBV	3438676	4241259	41.09%	5.568%
21	21.427	3115	3118	3125	rBV3	109305	141880	1.37%	0.186%
22	21.856	3189	3191	3196	rBV3	128926	164849	1.60%	0.216%
23	22.321	3268	3270	3276	rVB2	190134	243351	2.36%	0.319%
24	22.450	3287	3292	3298	rVB	1462614	1903945	18.45%	2.500%
25	22.827	3353	3356	3360	rVB	176290	235386	2.28%	0.309%
26	23.544	3471	3478	3486	rVB	2023799	3709390	35.94%	4.870%

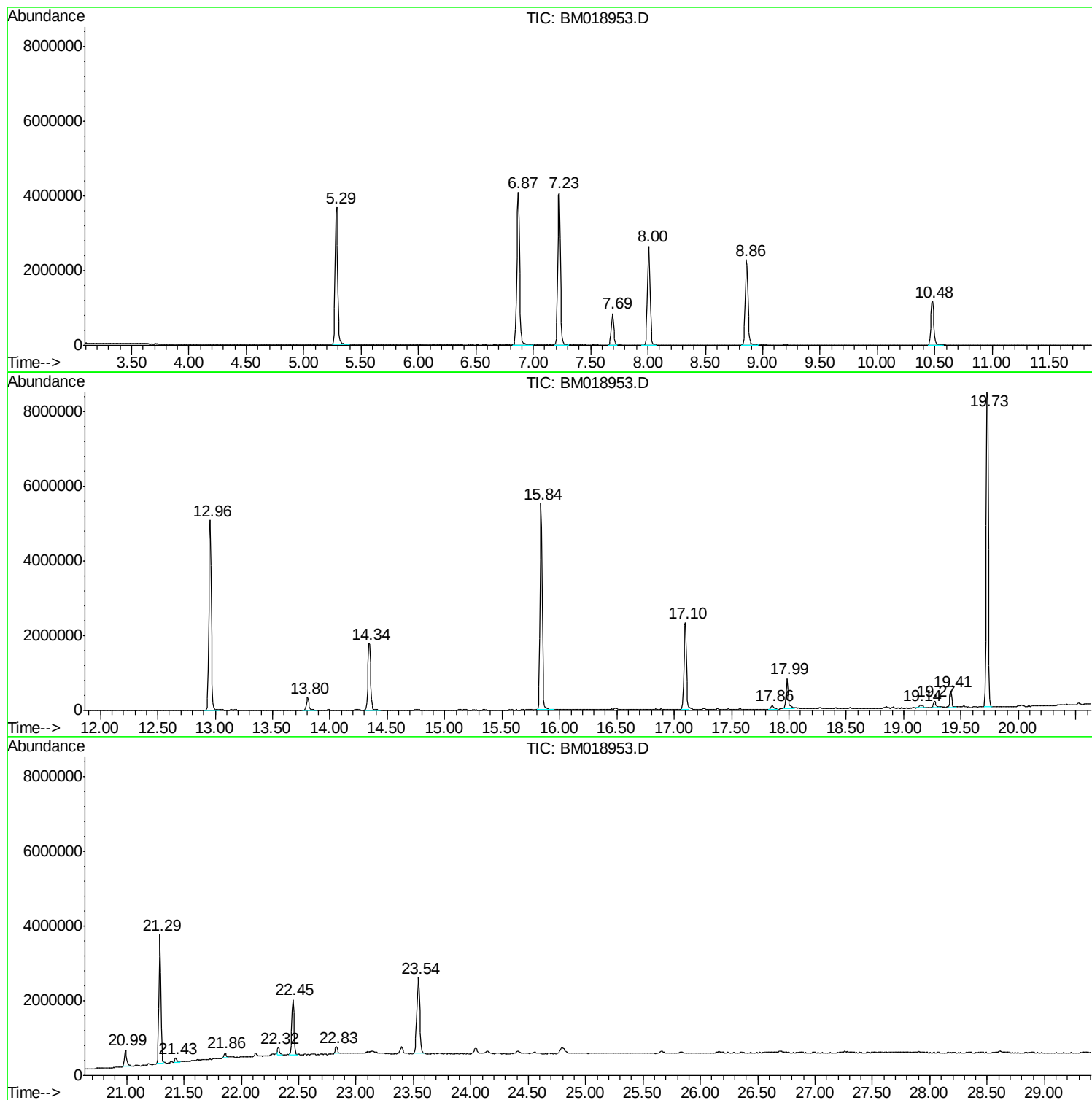
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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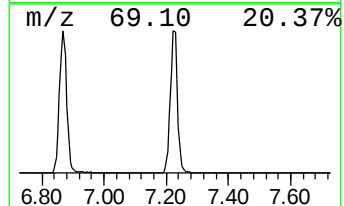
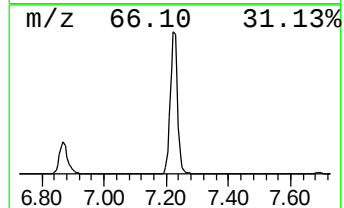
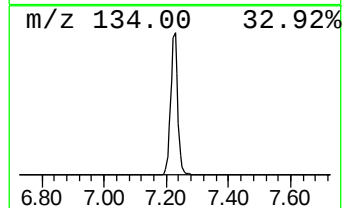
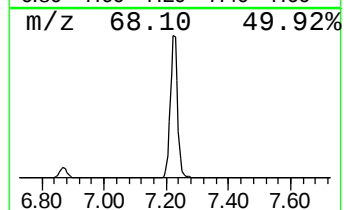
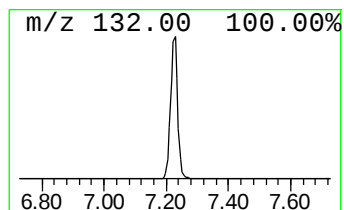
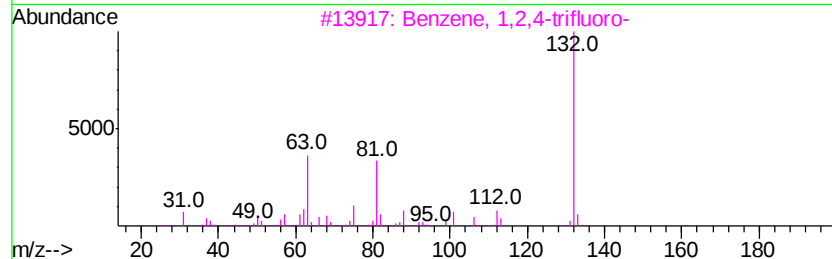
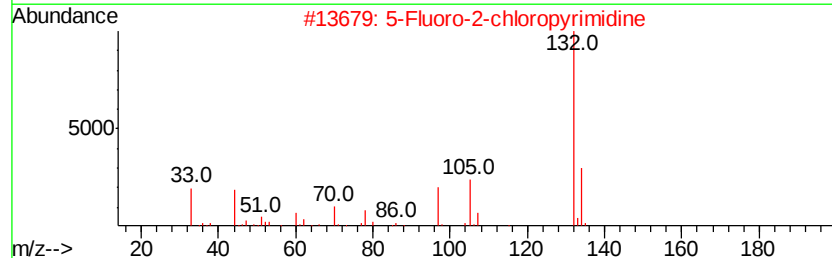
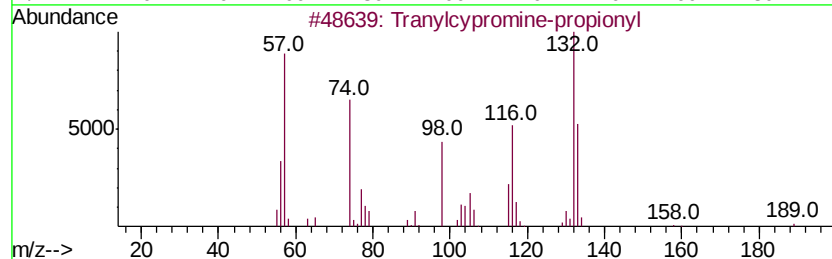
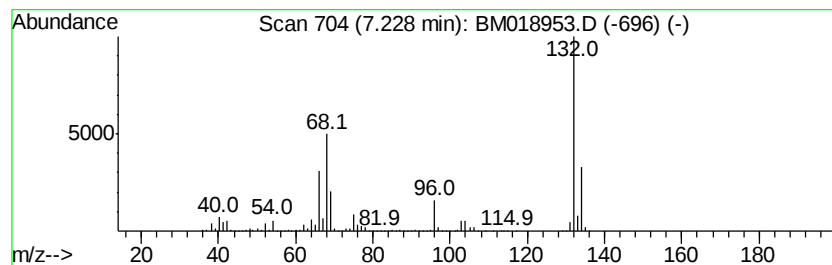
Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM021119.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown7.23 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	96.42 ng	6576550	1,4-Dichlorobenzene-d4	7.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranvlcypromine-propionyl	189	C12H15NO	1000123-86-3	12
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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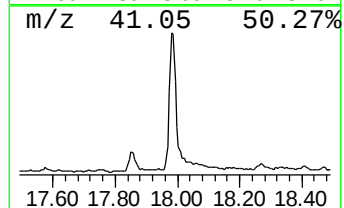
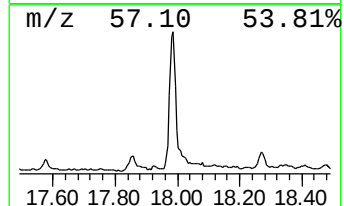
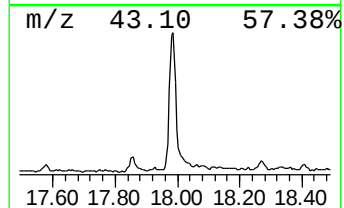
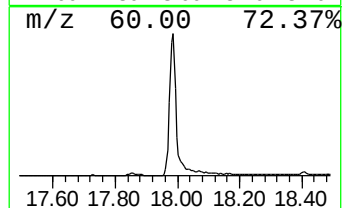
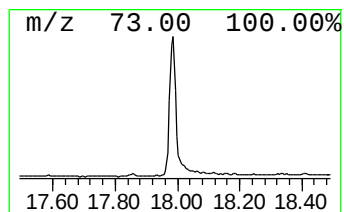
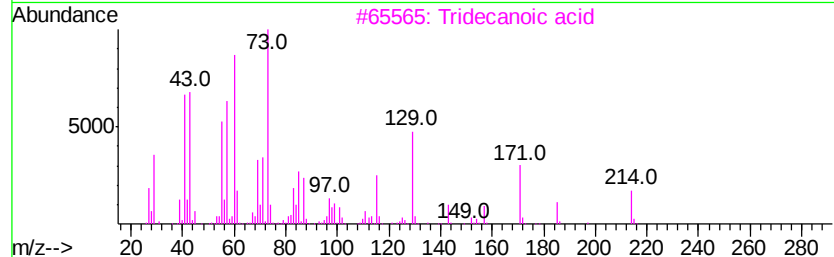
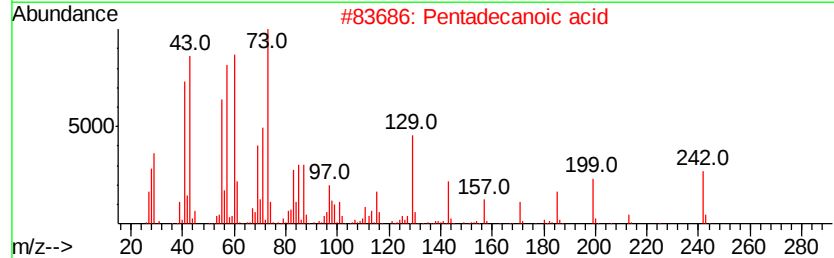
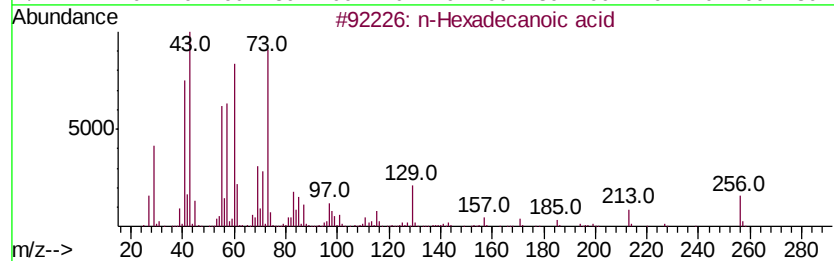
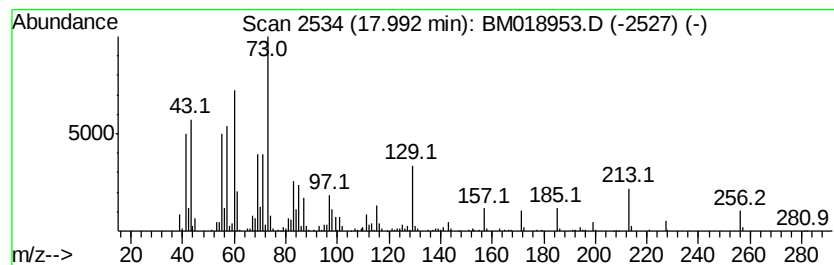
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
17.99	7.39 ng	1249720	Phenanthrene-d10	17.10	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	94
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	60
4	Hexadecane	226	C16H34	000544-76-3	18
5	Dodecane	170	C12H26	000112-40-3	18



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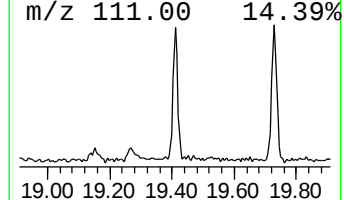
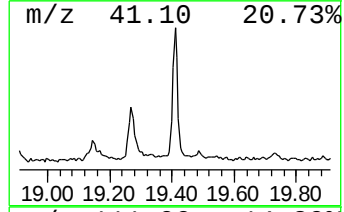
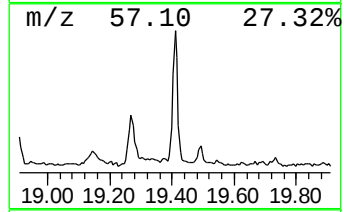
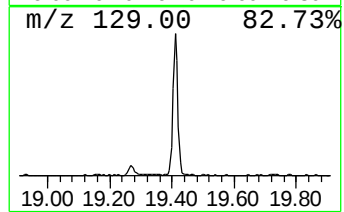
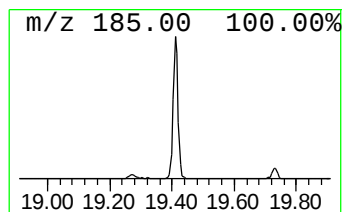
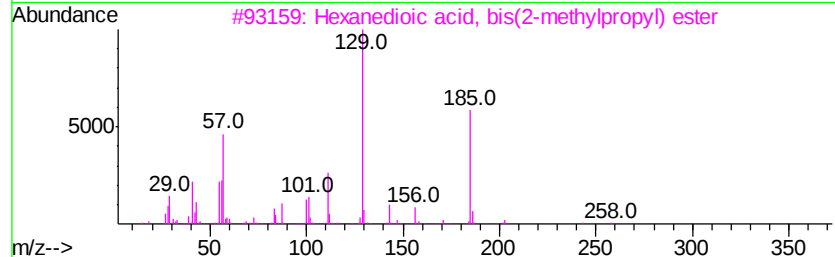
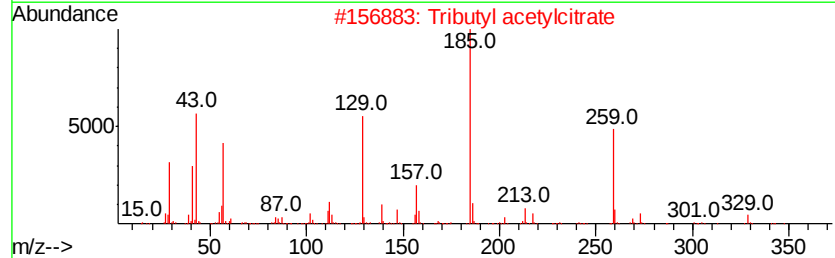
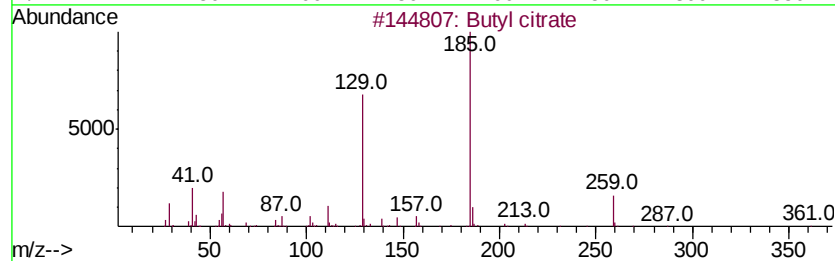
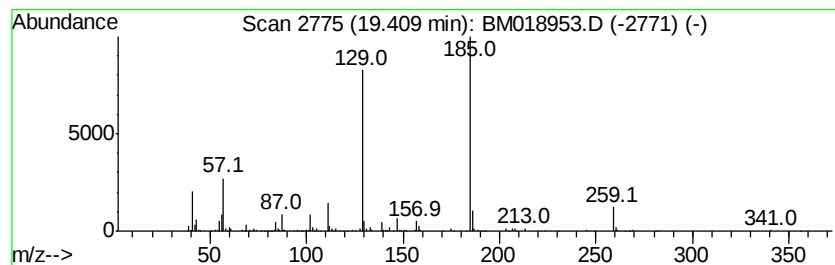
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 Peak Number 4 Butyl citrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.41	2.27 ng	481516	Chrysene-d12	21.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butyl citrate	360	C18H32O7	000077-94-1	91
2	Tributyl acetylcitrate	402	C20H34O8	000077-90-7	64
3	Hexanedioic acid, bis(2-methylpr...	258	C14H26O4	000141-04-8	56
4	Butanedioic acid, 2,3-dimethyl-,...	258	C14H26O4	056051-57-1	50
5	Resorufin	213	C12H7NO3	000635-78-9	35



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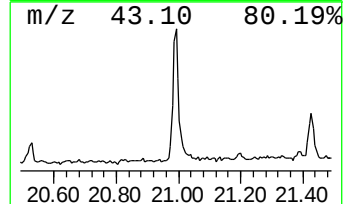
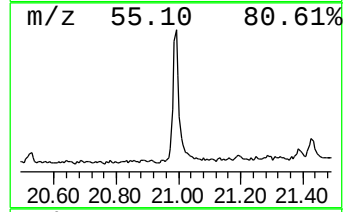
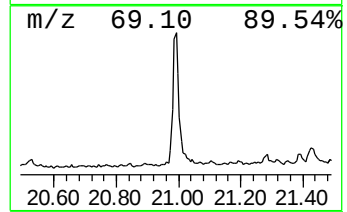
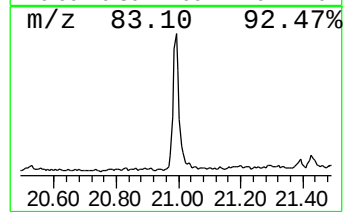
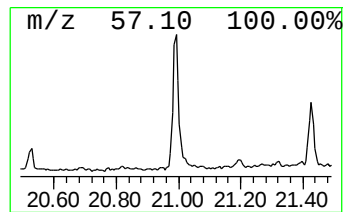
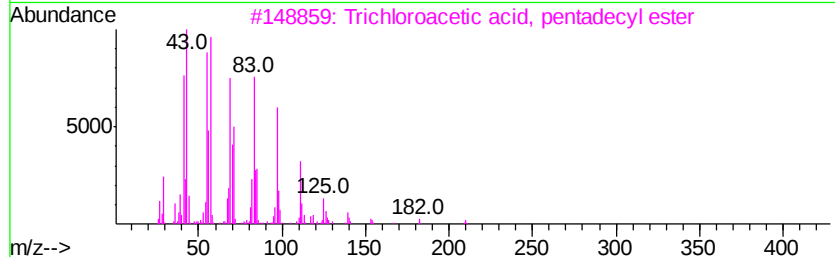
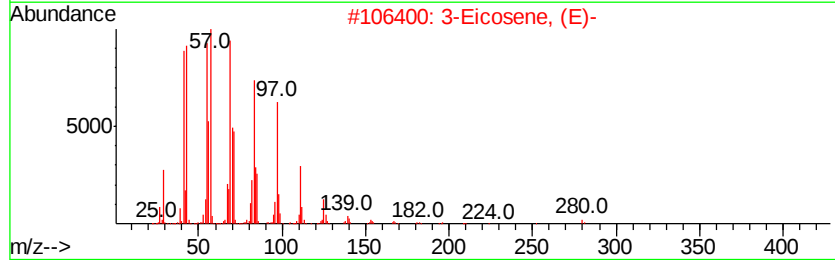
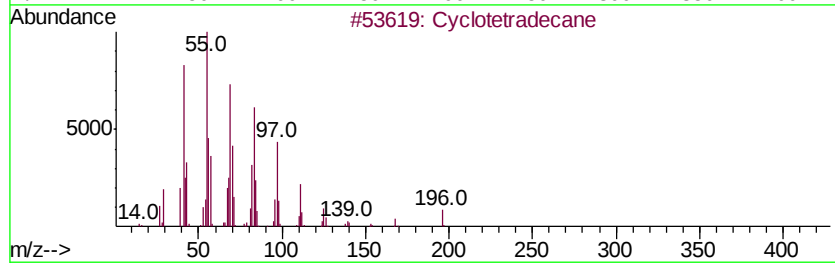
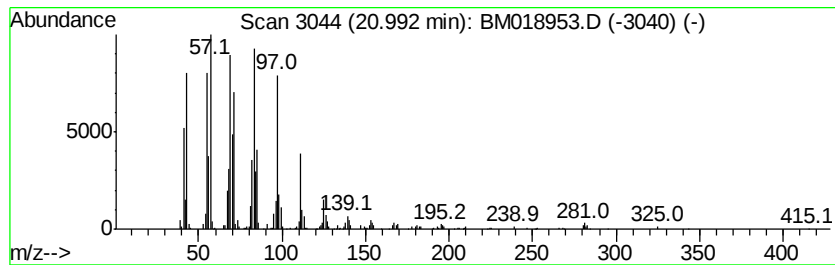
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Peak Number 5 Cyclotetradecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.99	2.83 ng	600631	Chrysene-d12	21.29	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cvcclotetradecane	196	C14H28	000295-17-0	94
2	3-Eicosene, (E)-	280	C20H40	074685-33-9	91
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
4	Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5	Heptafluorobutyric acid, n-penta...	424	C19H31F7O2	1000216-79-3	91



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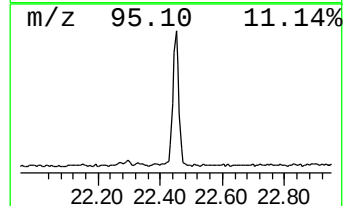
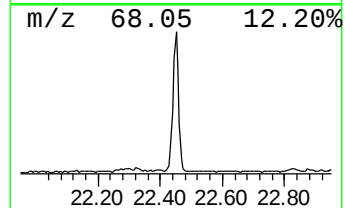
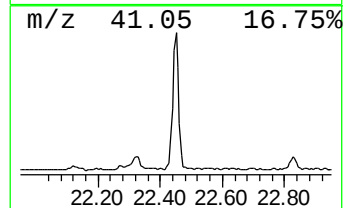
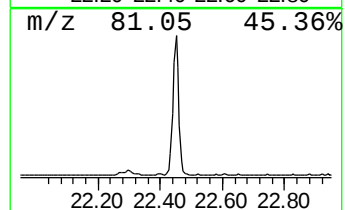
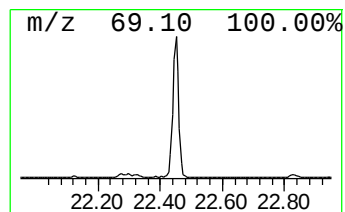
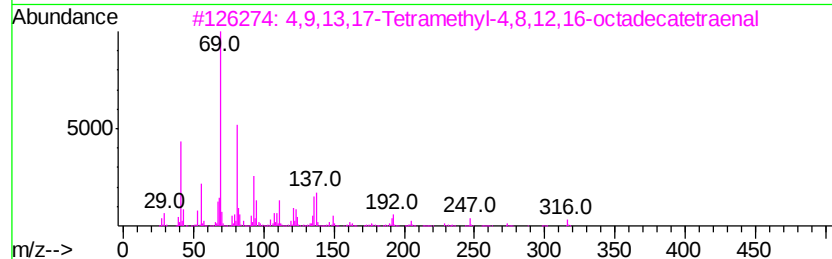
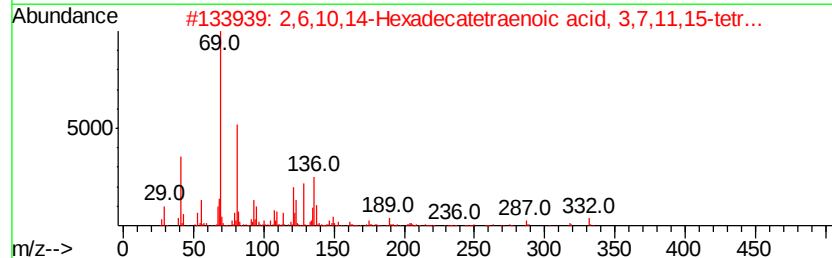
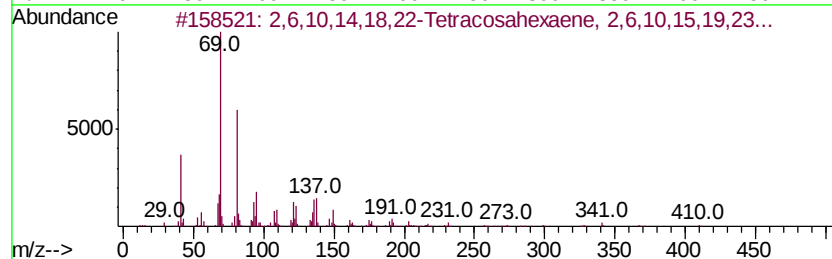
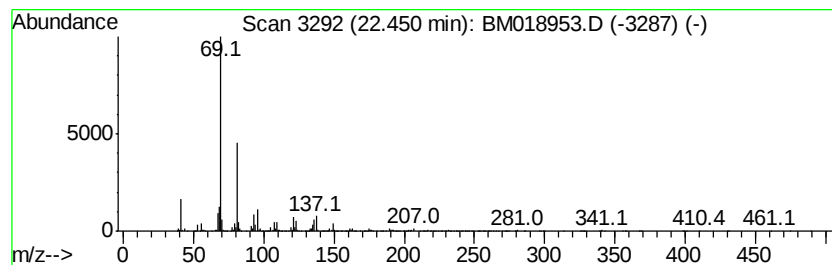
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Peak Number 6 2,6,10,14,18,22-Tetracosae... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.45	10.27 ng	1903950	Perylene-d12	23.54
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410 C30H50	000111-02-4	84
2	2,6,10,14-Hexadecatetraenoic aci...	332 C22H36O2	024035-35-6	83
3	4,9,13,17-Tetramethyl-4,8,12,16-...	316 C22H36O	056882-09-8	83
4	7,11-Dimethyldodeca-2,6,10-trien...	208 C14H24O	125529-10-4	72
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222 C15H26O	004602-84-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.23	7.23	96.4	ng	6576550	1	7.69	1364190	20.0
n-Hexadecanoic acid	17.99	7.4	ng	1249720	4	17.10	3381570	20.0
Butyl citrate	19.41	2.3	ng	481516	5	21.29	4241260	20.0
Cyclotetradecane	20.99	2.8	ng	600631	5	21.29	4241260	20.0
2,6,10,14,18,22-T...	22.45	10.3	ng	1903950	6	23.54	3709390	20.0