

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM012021\
 Data File : BM028474.D
 Acq On : 20 Jan 2021 18:55
 Operator : CG/JU
 Sample : M1160-05
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 BASIN-2

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-BM012021.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM028474.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.551	396	402	412	rVB	447898	668054	71.63%	10.348%
2	7.192	673	681	691	rVB	427474	697053	74.74%	10.798%
3	8.034	818	824	830	rBV	126620	198324	21.26%	3.072%
4	9.204	1015	1023	1032	rBV	273210	437679	46.93%	6.780%
5	10.845	1296	1302	1311	rBV	155435	261015	27.99%	4.043%
6	13.298	1712	1719	1725	rVB	570998	808550	86.69%	12.525%
7	14.121	1854	1859	1865	rBV	11761	15242	1.63%	0.236%
8	14.504	1915	1924	1930	rBV3	5679	12942	1.39%	0.200%
9	14.668	1946	1952	1959	rBV	203092	301103	32.28%	4.664%
10	16.151	2198	2204	2210	rBV	439036	597052	64.01%	9.248%
11	17.398	2410	2416	2422	rBV	230855	319940	34.30%	4.956%
12	18.268	2559	2564	2570	rBV	52326	79175	8.49%	1.226%
13	19.027	2688	2693	2697	rBV	49528	62747	6.73%	0.972%
14	19.115	2704	2708	2712	rBV	13491	16883	1.81%	0.262%
15	19.533	2776	2779	2786	rBV6	12502	21411	2.30%	0.332%
16	19.650	2795	2799	2803	rBV	15207	21085	2.26%	0.327%
17	19.986	2851	2856	2864	rBV	746895	932678	100.00%	14.447%
18	20.656	2967	2970	2973	rVB	17052	19004	2.04%	0.294%
19	20.856	3001	3004	3008	rBV	82834	94703	10.15%	1.467%
20	20.903	3010	3012	3016	rVB	15821	16970	1.82%	0.263%
21	21.227	3063	3067	3072	rBV	123530	155648	16.69%	2.411%
22	21.527	3113	3118	3126	rBV	291128	354232	37.98%	5.487%
23	23.815	3502	3507	3514	rVB2	194381	364197	39.05%	5.641%

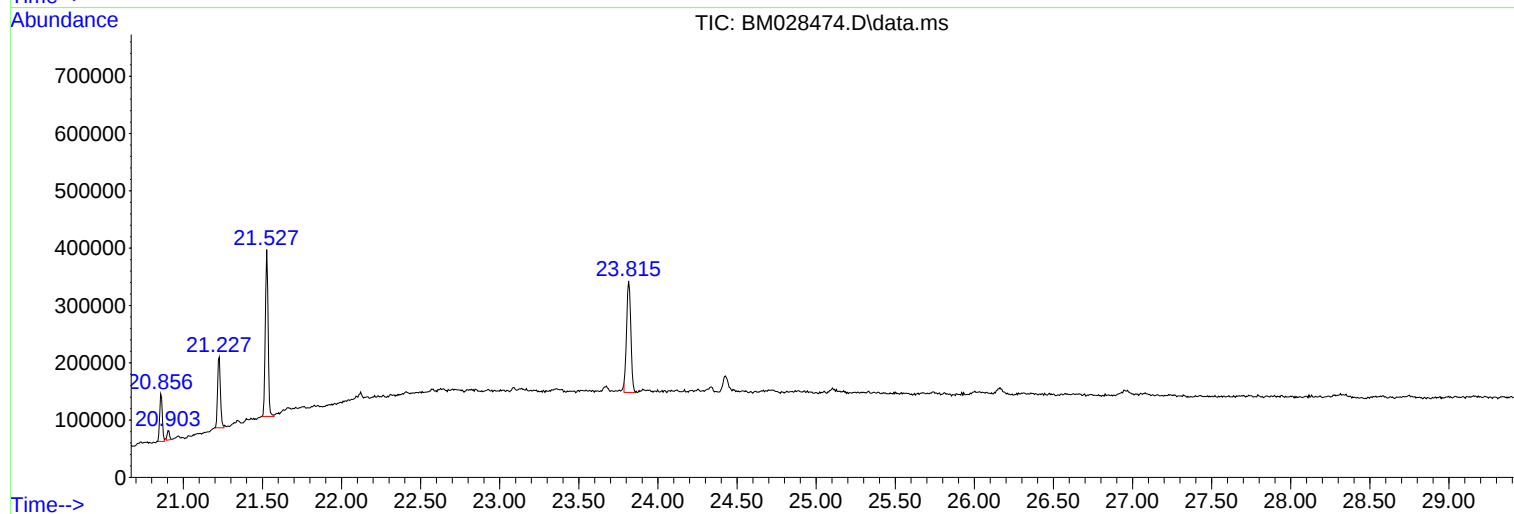
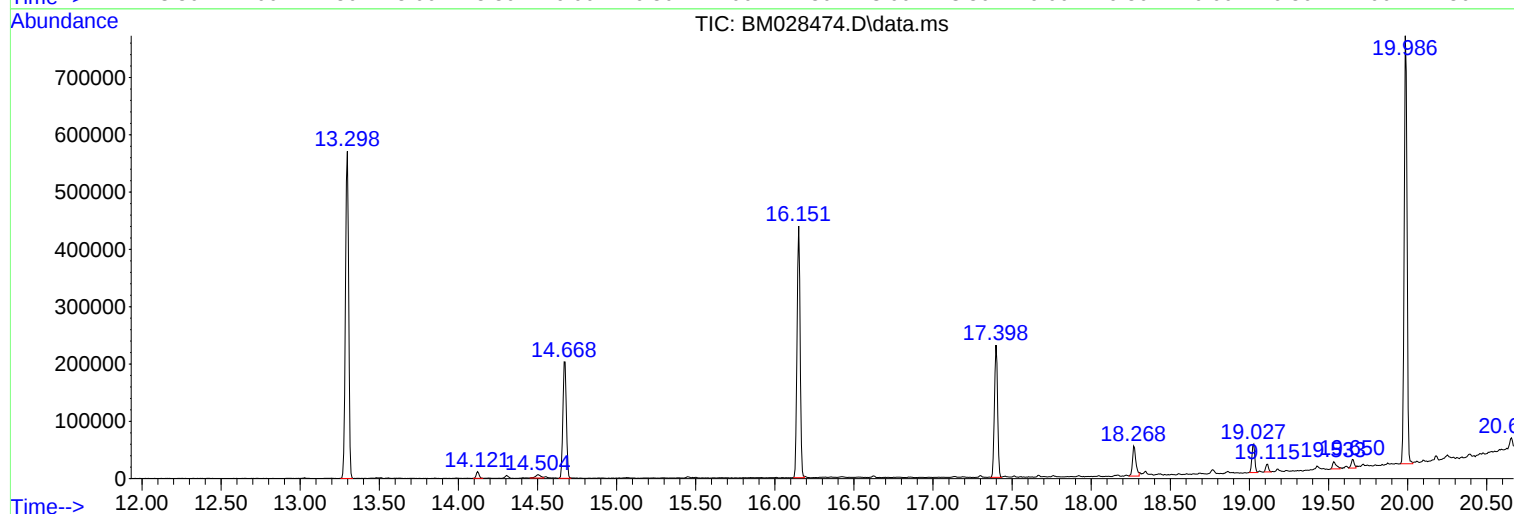
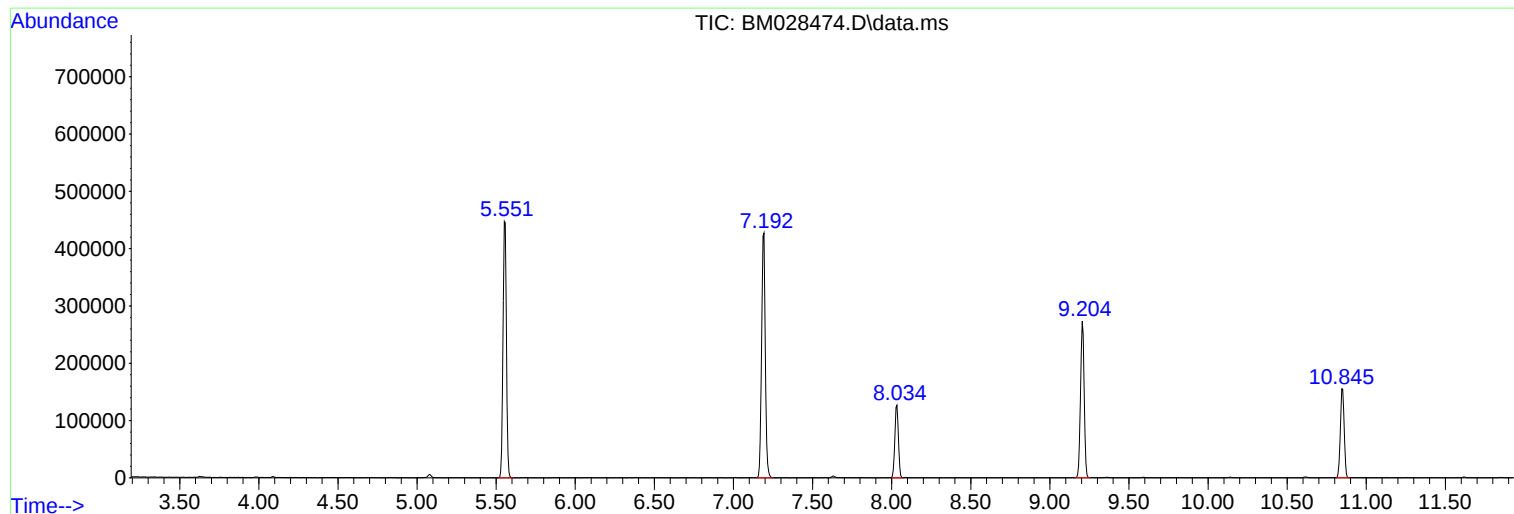
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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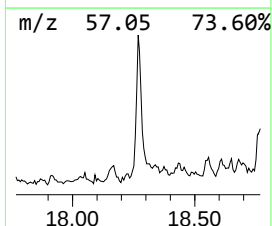
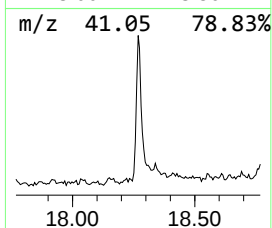
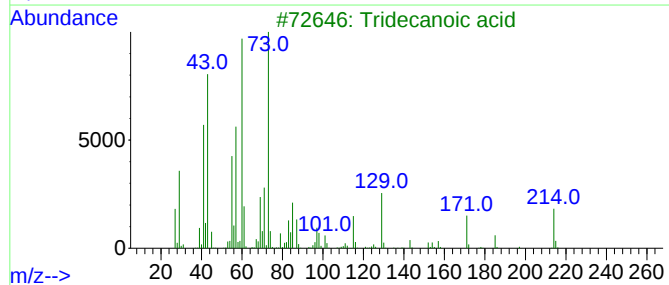
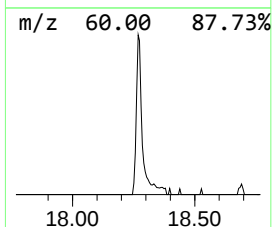
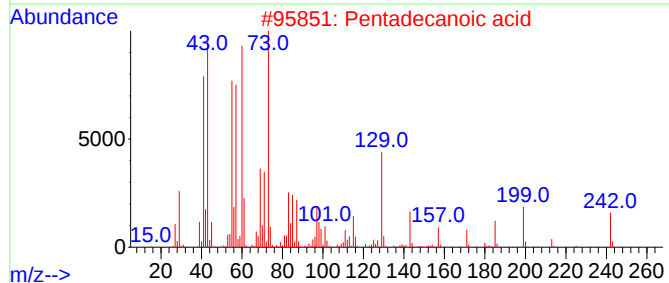
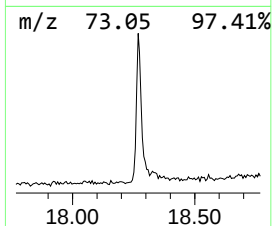
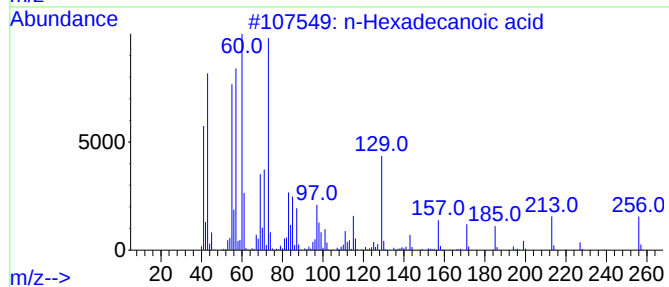
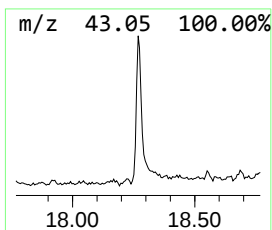
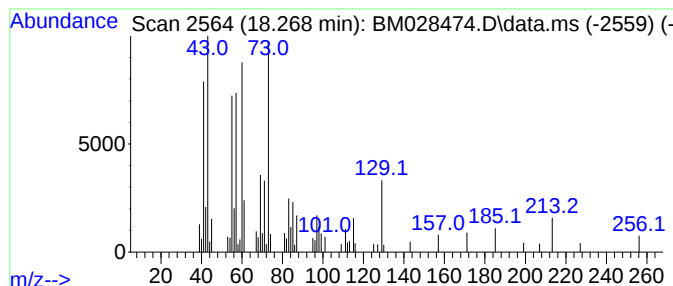
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM012021.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.268	4.95 ng	79175	Phenanthrene-d10	17.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tridecanoic acid	214	C13H26O2	000638-53-9	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5			Dodecanoic acid	200	C12H24O2	000143-07-7	59



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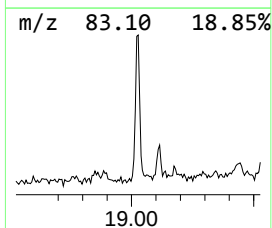
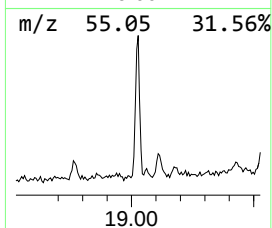
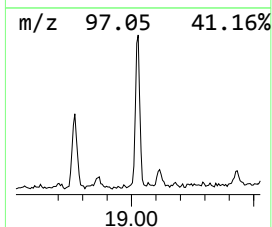
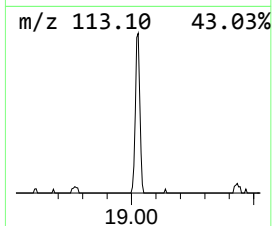
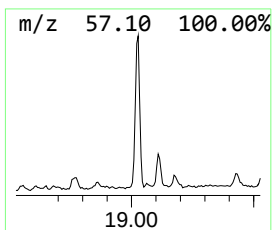
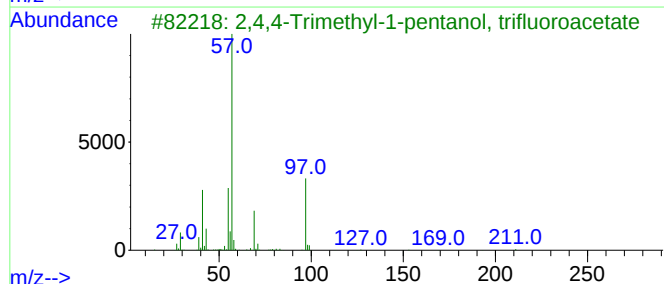
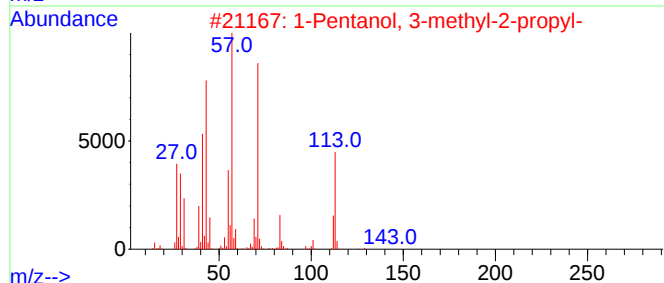
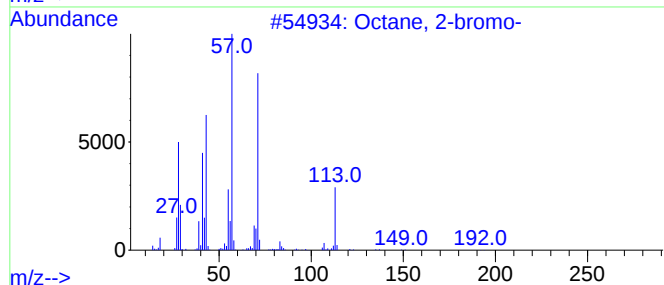
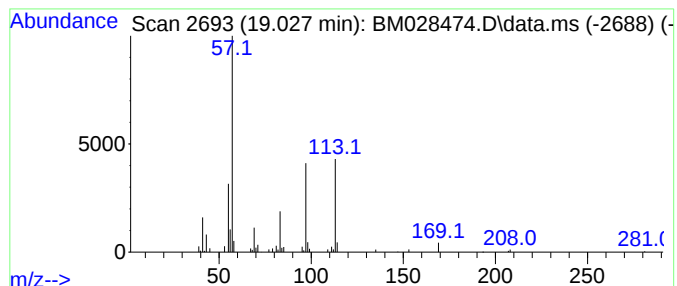
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Peak Number 2 unknown19.027 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.027	3.92 ng	62747	Phenanthrene-d10	17.398

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octane, 2-bromo-		192	C8H17Br		000557-35-7	47
2	1-Pentanol, 3-methyl-2-propyl-		144	C9H20O		054004-40-9	40
3	2,4,4-Trimethyl-1-pentanol, trif...		226	C10H17F3O2		1000365-19-5	38
4	2,4,4-Trimethyl-1-pentanol, pent...		276	C11H17F5O2		1000365-51-0	37
5	2,4,4,6,6,8,8-Heptamethyl-1-nonene		224	C16H32		015796-04-0	37



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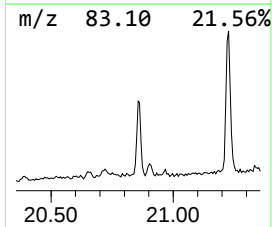
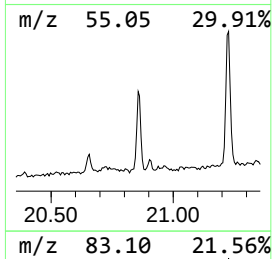
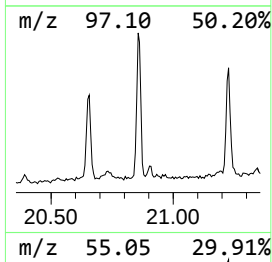
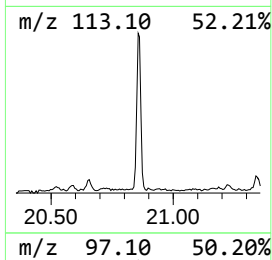
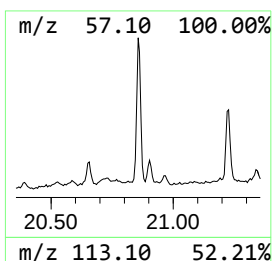
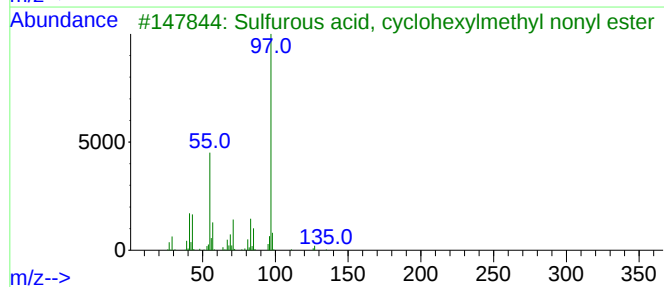
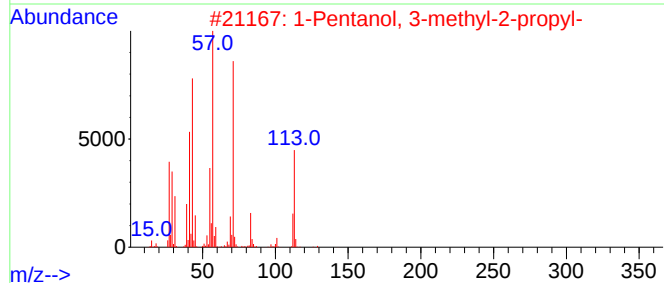
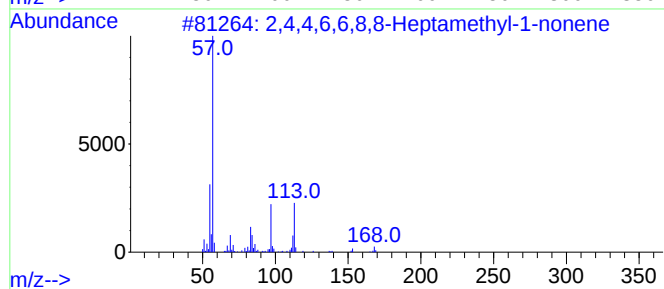
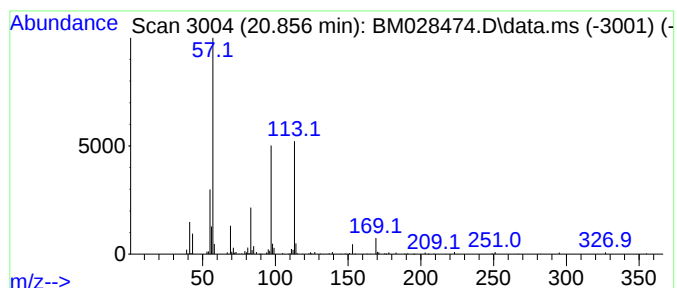
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Peak Number 3 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.856	5.35 ng	94703	Chrysene-d12	21.527

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	64	
2	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	37	
3	Sulfurous acid, cyclohexylmethyl...	304	C16H32O3S	1000309-21-8	32	
4	Octane, 2-bromo-	192	C8H17Br	000557-35-7	25	
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25	



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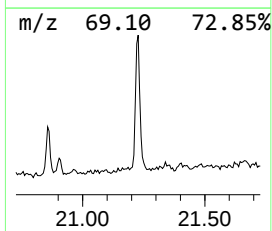
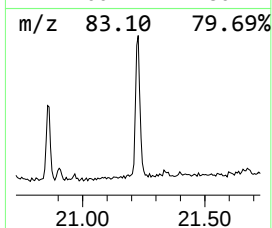
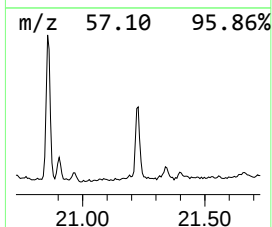
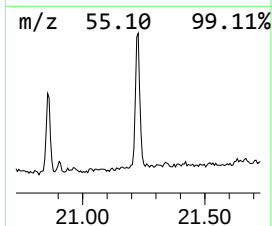
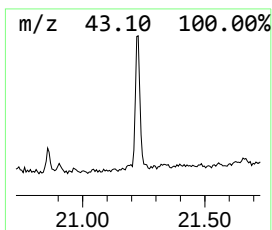
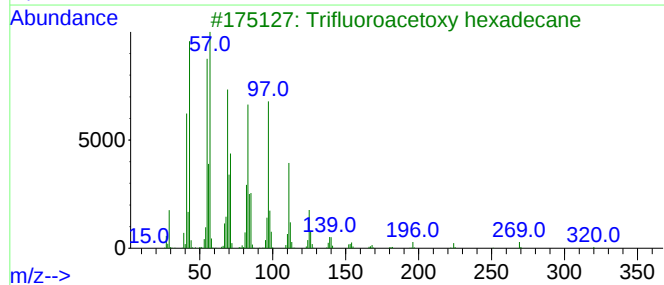
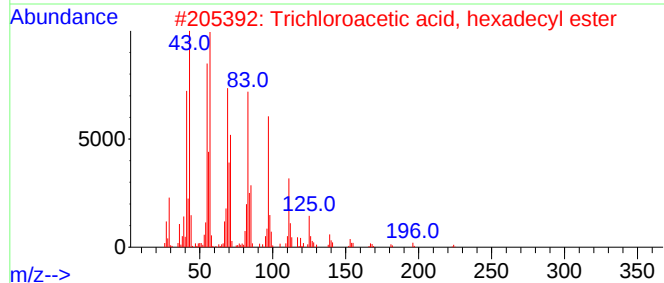
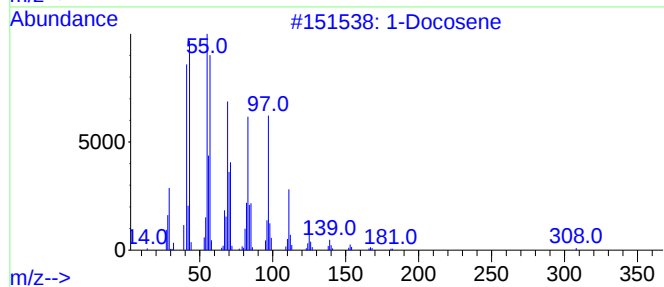
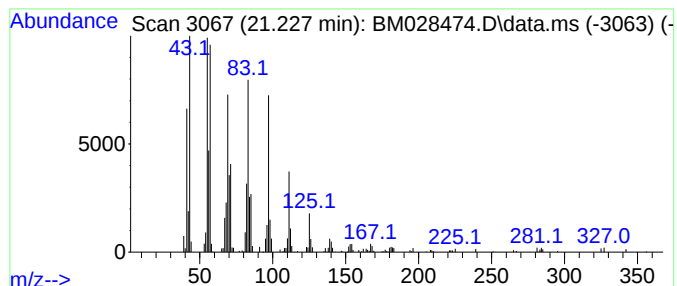
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Peak Number 4 1-Docosene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.227	8.79 ng	155648	Chrysene-d12	21.527

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Docosene			308	C22H44	001599-67-3	95
2	Trichloroacetic acid, hexadecyl ...			386	C18H33Cl3O2	074339-54-1	94
3	Trifluoroacetoxy hexadecane			338	C18H33F3O2	006222-03-3	94
4	1-Heneicosanol			312	C21H44O	015594-90-8	93
5	Pentafluoropropionic acid, penta...			374	C18H31F5O2	959092-08-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	18.268	5.0	ng	79175	4	17.398	319940	20.0
unknown19.027	19.027	3.9	ng	62747	4	17.398	319940	20.0
2,4,4,6,6,8,8-H...	20.856	5.3	ng	94703	5	21.527	354232	20.0
1-Docosene	21.227	8.8	ng	155648	5	21.527	354232	20.0