

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042221\
 Data File : BP005373.D
 Acq On : 22 Apr 2021 13:43
 Operator : CG/JU
 Sample : M2023-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 FK-GF-02-070-A

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_P\Methods\8270E-BP042121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.246	360	367	379	rBV	739854	1042271	41.11%	8.227%
2	6.834	629	637	653	rBV	678862	1095573	43.21%	8.648%
3	7.640	766	774	782	rBV	158831	250132	9.87%	1.974%
4	8.805	964	972	987	rBV	424017	688718	27.17%	5.436%
5	10.428	1241	1248	1256	rBV	177378	300909	11.87%	2.375%
6	12.916	1664	1671	1685	rBV	945197	1354030	53.41%	10.688%
7	13.769	1811	1816	1824	rBV	17874	30217	1.19%	0.239%
8	14.304	1900	1907	1915	rBV2	275300	393442	15.52%	3.106%
9	15.810	2155	2163	2182	rBV	899102	1349991	53.25%	10.656%
10	17.069	2370	2377	2381	rBV	360291	519946	20.51%	4.104%
11	17.110	2381	2384	2390	rVB	48503	69698	2.75%	0.550%
12	17.204	2395	2400	2405	rVB	23289	37274	1.47%	0.294%
13	17.969	2526	2530	2539	rVB2	105715	153878	6.07%	1.215%
14	18.134	2553	2558	2562	rBV3	21583	36170	1.43%	0.285%
15	18.439	2606	2610	2614	rBV3	18501	27373	1.08%	0.216%
16	18.698	2650	2654	2658	rBV	71272	84150	3.32%	0.664%
17	19.092	2716	2721	2729	rVB	225394	288709	11.39%	2.279%
18	19.210	2738	2741	2751	rBV4	51562	77262	3.05%	0.610%
19	19.416	2773	2776	2777	rBV	30183	34886	1.38%	0.275%
20	19.445	2777	2781	2785	rVB	154320	182269	7.19%	1.439%
21	19.645	2810	2815	2820	rBV	2241013	2535212	100.00%	20.011%
22	20.028	2877	2880	2885	rBV2	29285	48392	1.91%	0.382%
23	20.510	2958	2962	2966	rBV	127627	158168	6.24%	1.248%
24	20.886	3022	3026	3033	rVB3	167796	240211	9.47%	1.896%
25	21.169	3068	3074	3078	rBV2	607908	908914	35.85%	7.174%
26	21.204	3078	3080	3086	rVB	118273	151182	5.96%	1.193%
27	23.427	3453	3458	3464	rVB2	342734	610083	24.06%	4.816%

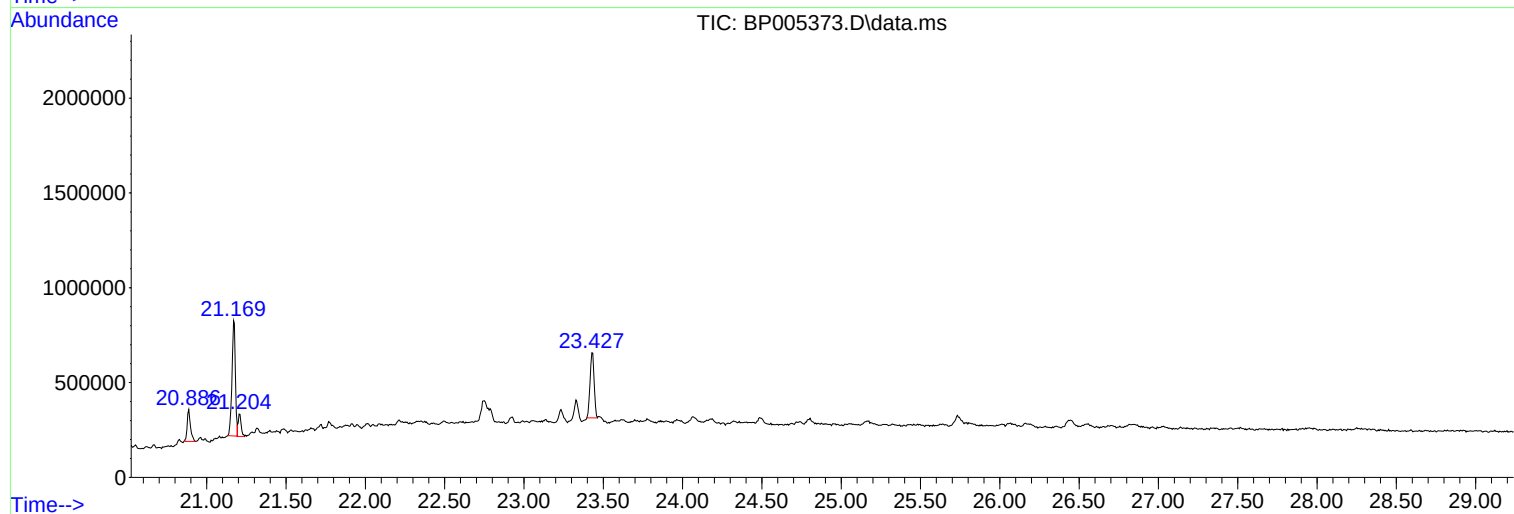
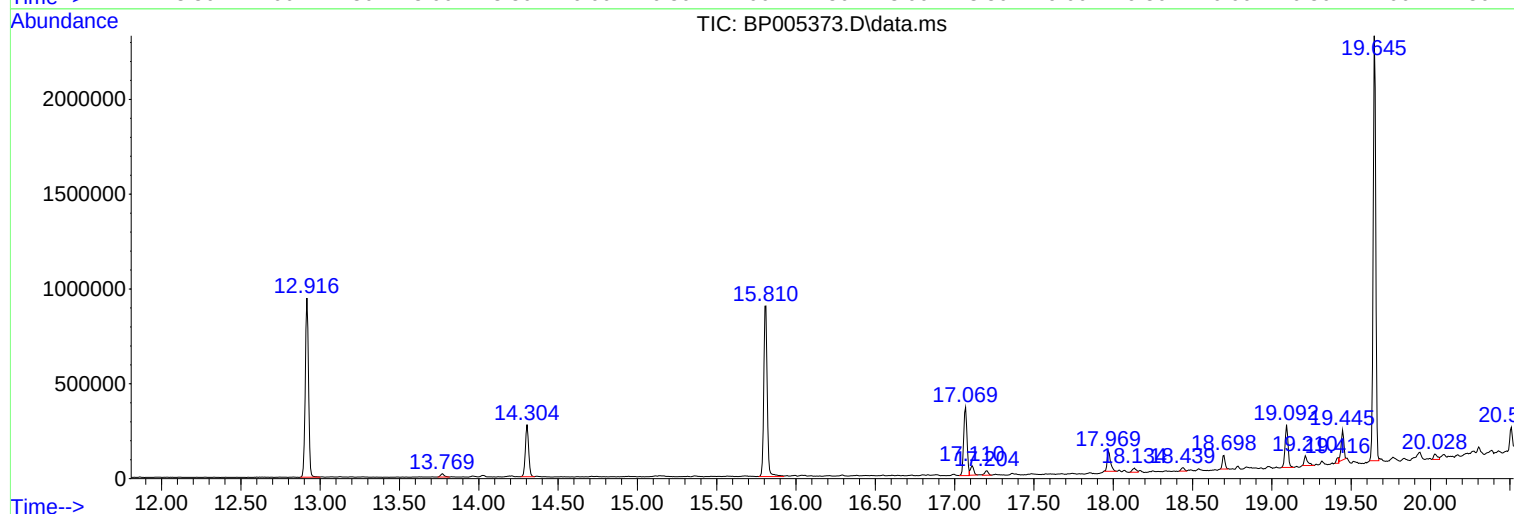
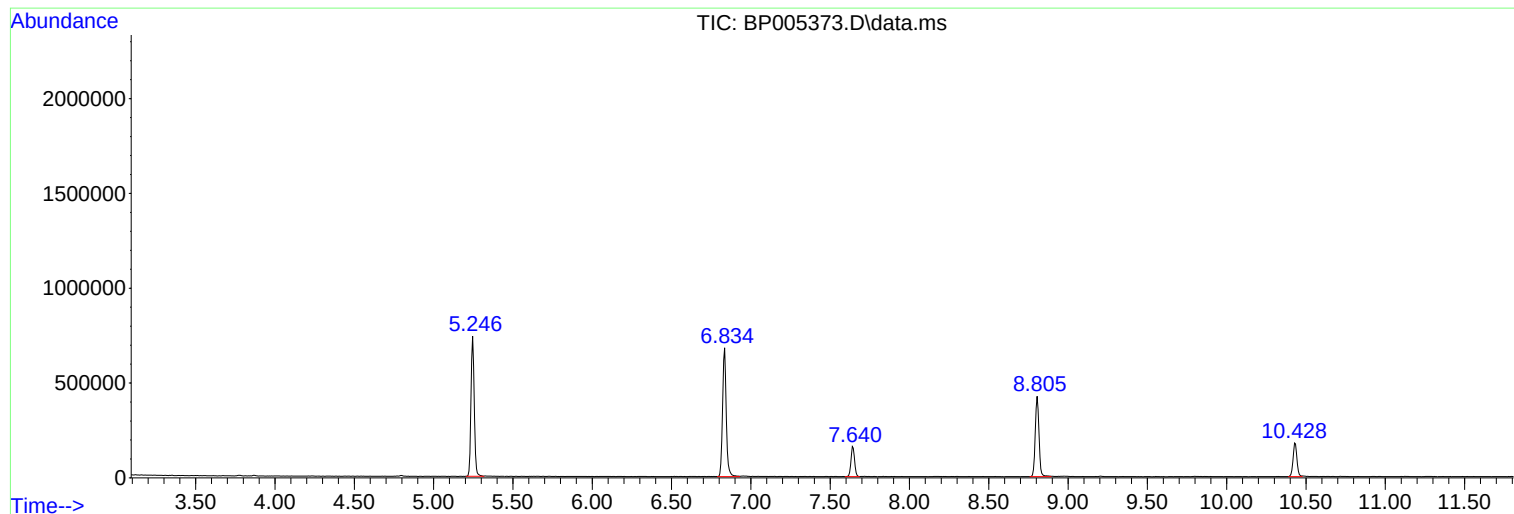
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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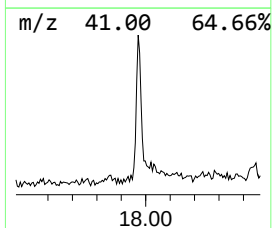
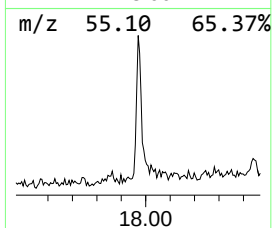
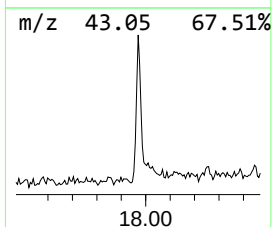
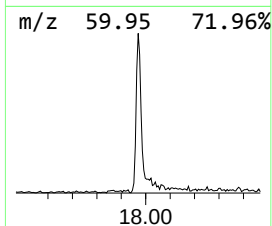
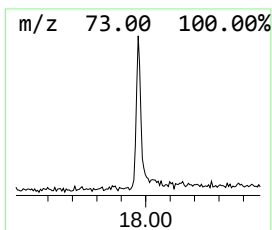
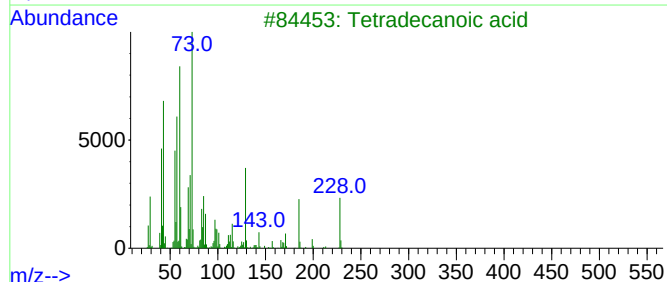
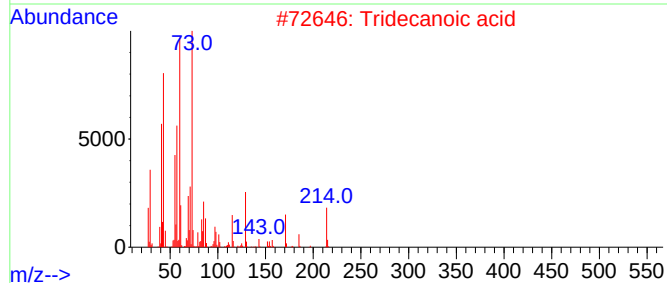
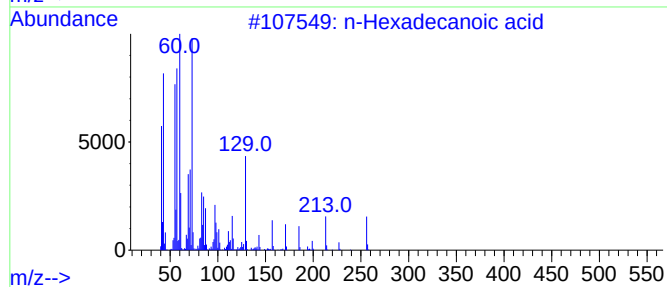
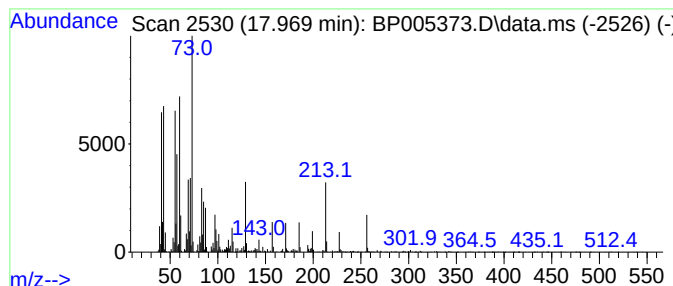
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP042121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.969	5.92 ng	153878	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2			Tridecanoic acid	214	C13H26O2	000638-53-9	83
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	49



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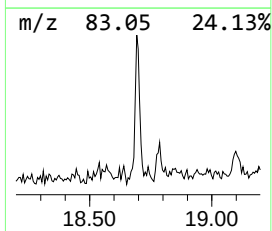
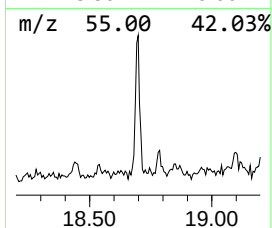
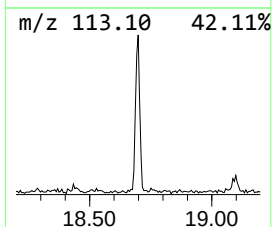
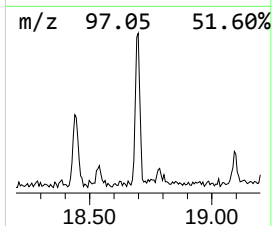
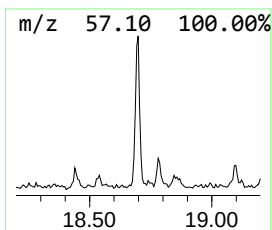
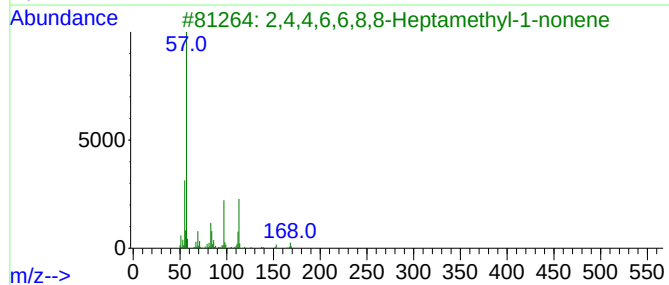
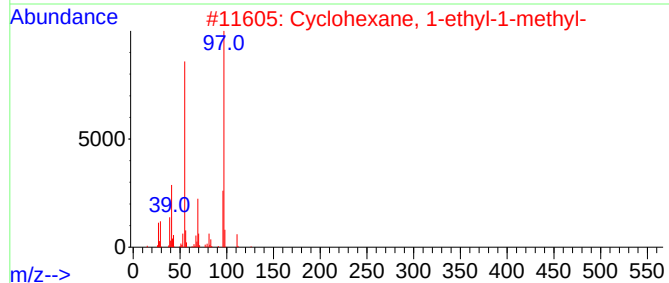
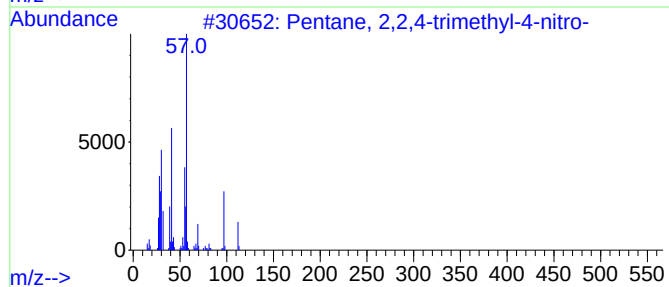
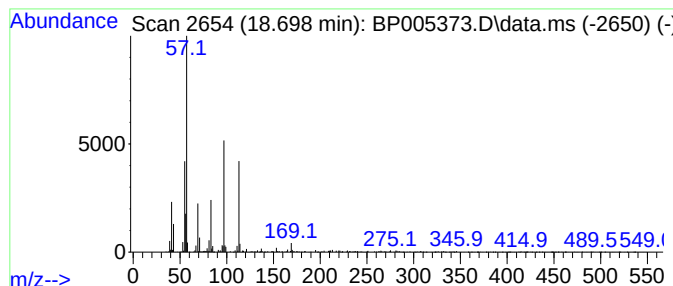
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Peak Number 2 unknown18.69 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.698	3.24 ng	84150	Phenanthrene-d10	17.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-4-nitro-	159	C8H17NO2	005342-78-9	38
2			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	22
3			2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	17
4			4-Methylnonanoic acid	172	C10H20O2	045019-28-1	17
5			2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	17



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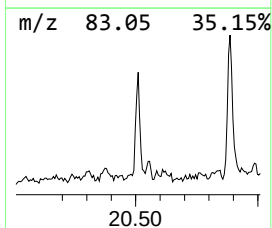
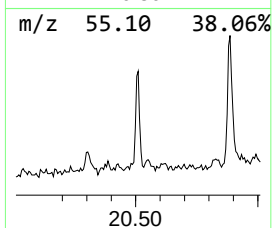
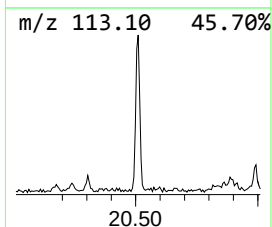
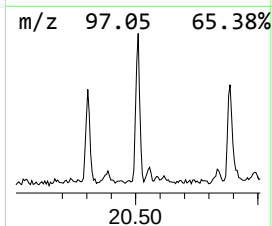
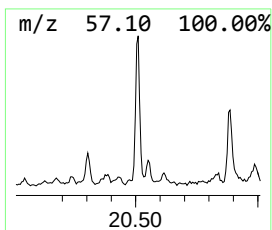
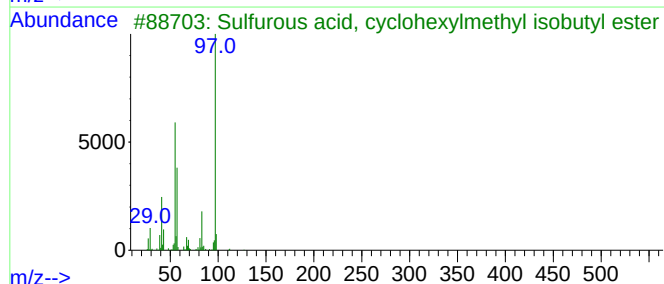
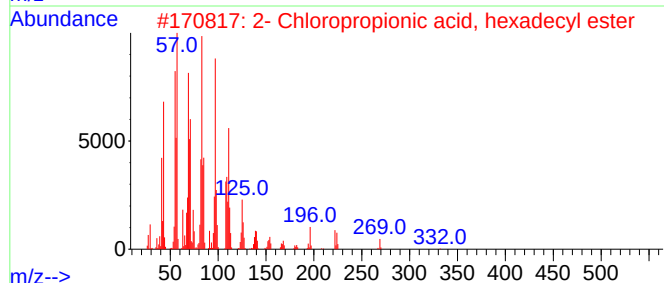
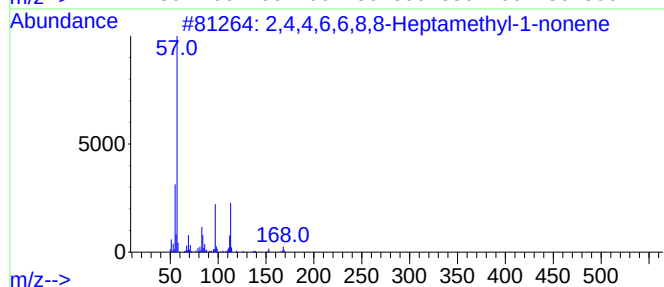
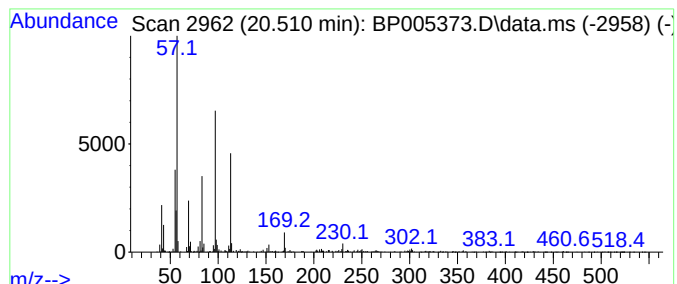
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Peak Number 3 unknown20.51 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.510	3.48 ng	158168	Chrysene-d12	21.175

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	45		
2	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	27		
3	Sulfurous acid, cyclohexylmethyl...	234	C11H22O3S	1000309-21-3	25		
4	Sulfurous acid, cyclohexylmethyl...	416	C24H48O3S	1000309-22-5	16		
5	Sulfurous acid, cyclohexylmethyl...	262	C13H26O3S	1000309-21-5	12		



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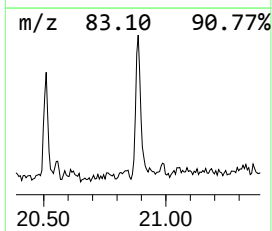
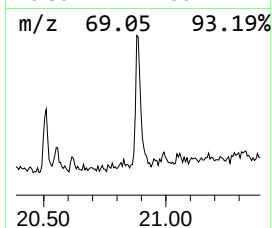
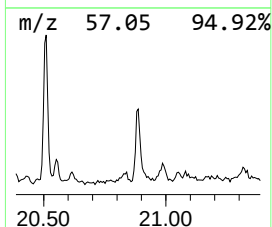
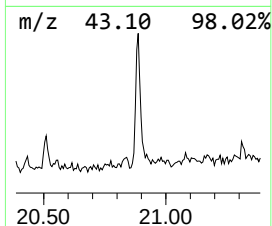
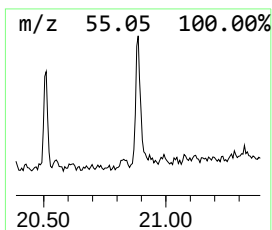
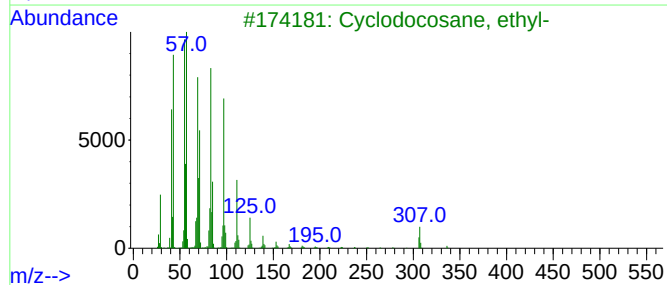
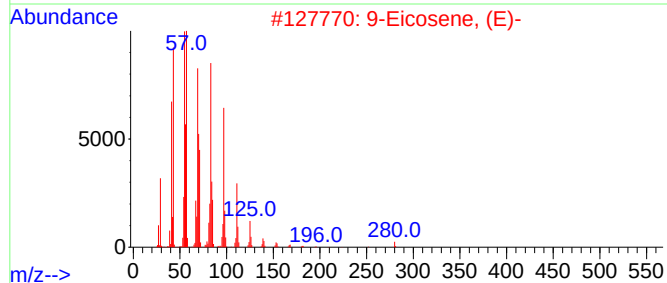
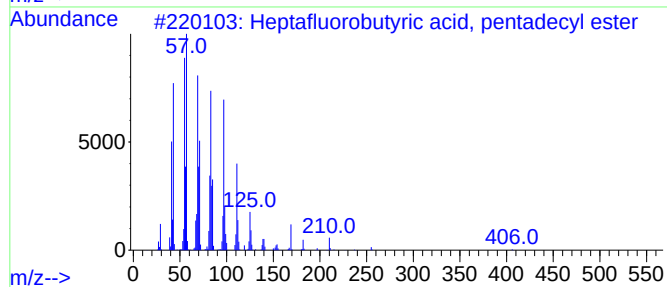
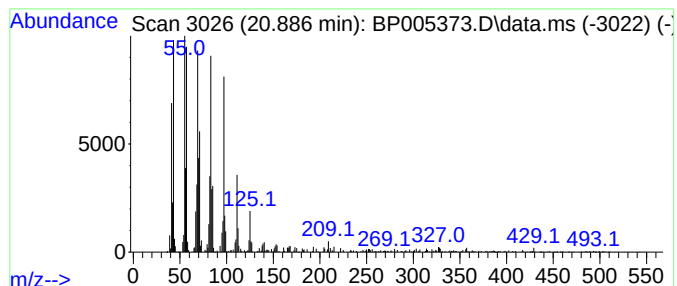
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Peak Number 4 Heptafluorobutyric acid, pe... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.886	5.29 ng	240211	Chrysene-d12	21.175

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
2			9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3			Cyclodocosane, ethyl-	336	C24H48	1000151-22-6	91
4			9-Tricosene, (Z)-	322	C23H46	027519-02-4	90
5			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.969	5.9	ng	153878	4	17.069	519946	20.0
unknown18.69	18.698	3.2	ng	84150	4	17.069	519946	20.0
unknown20.51	20.510	3.5	ng	158168	5	21.175	908914	20.0
Heptafluorobuty...	20.886	5.3	ng	240211	5	21.175	908914	20.0