

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062223\
 Data File : BG057819.D
 Acq On : 22 Jun 2023 22:21
 Operator : CG/JU
 Sample : 03302-03
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-4

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-BG061923.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG057819.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.027	323	330	337	rBV	285103	409873	18.59%	3.540%
2	5.491	402	409	420	rVB	539700	820237	37.20%	7.085%
3	7.078	671	679	691	rBV	564883	948148	43.00%	8.190%
4	7.918	816	822	831	rBV	114123	190940	8.66%	1.649%
5	9.081	1012	1020	1029	rBV	312632	536949	24.35%	4.638%
6	10.721	1292	1299	1308	rBV	172033	296471	13.44%	2.561%
7	13.177	1710	1717	1724	rBV	807080	1239386	56.21%	10.705%
8	14.551	1945	1951	1959	rVB	278918	442923	20.09%	3.826%
9	15.909	2175	2182	2190	rVB	178629	247989	11.25%	2.142%
10	16.038	2197	2204	2214	rBV	807919	1190182	53.97%	10.280%
11	16.473	2271	2278	2283	rVB	37267	52355	2.37%	0.452%
12	17.295	2412	2418	2429	rVB	412822	618285	28.04%	5.340%
13	18.188	2563	2570	2582	rBV	93519	159449	7.23%	1.377%
14	19.463	2783	2787	2792	rBV2	18680	28603	1.30%	0.247%
15	19.916	2858	2864	2869	rBV	1652375	2205116	100.00%	19.047%
16	20.715	2995	3000	3004	rBV4	17530	23839	1.08%	0.206%
17	21.161	3071	3076	3079	rBV	27327	53146	2.41%	0.459%
18	21.202	3079	3083	3092	rVV2	172450	303583	13.77%	2.622%
19	21.285	3092	3097	3103	rVB	107801	148408	6.73%	1.282%
20	21.549	3135	3142	3150	rBV	428779	690728	31.32%	5.966%
21	21.749	3172	3176	3182	rVB3	22290	30097	1.36%	0.260%
22	22.348	3272	3278	3286	rBV5	22286	49522	2.25%	0.428%
23	23.024	3388	3393	3396	rBV4	14544	25431	1.15%	0.220%
24	23.811	3523	3527	3533	rVB6	13689	23938	1.09%	0.207%
25	24.692	3667	3677	3691	rVB	264294	772134	35.02%	6.669%
26	25.962	3887	3893	3903	rVB5	24928	69763	3.16%	0.603%

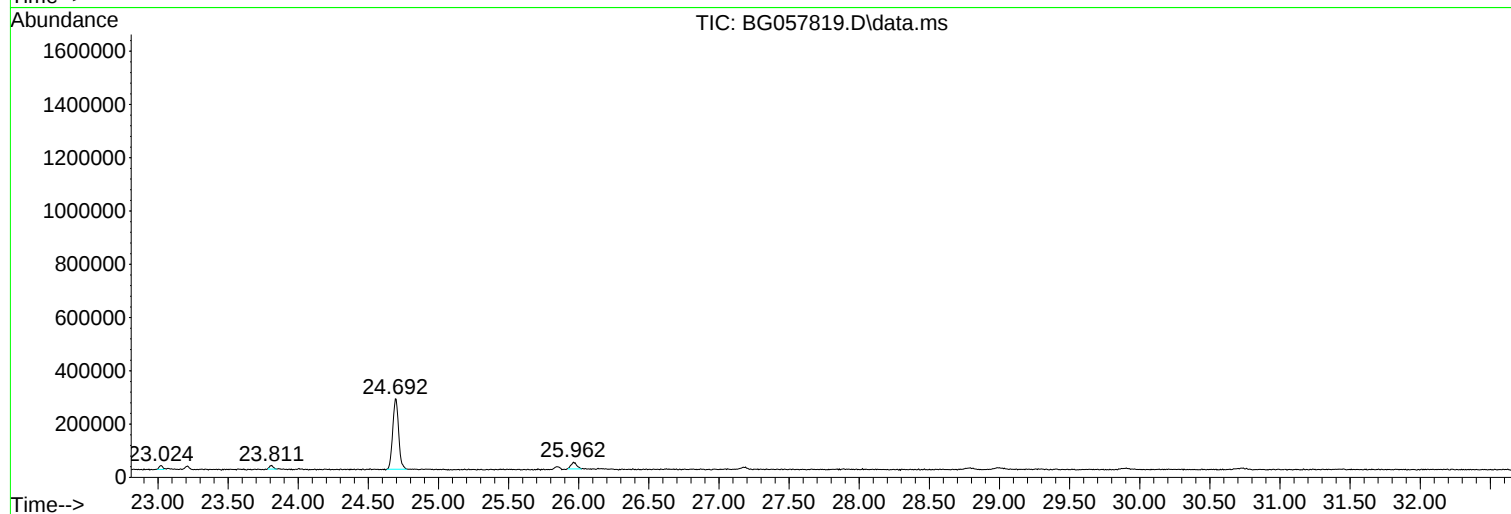
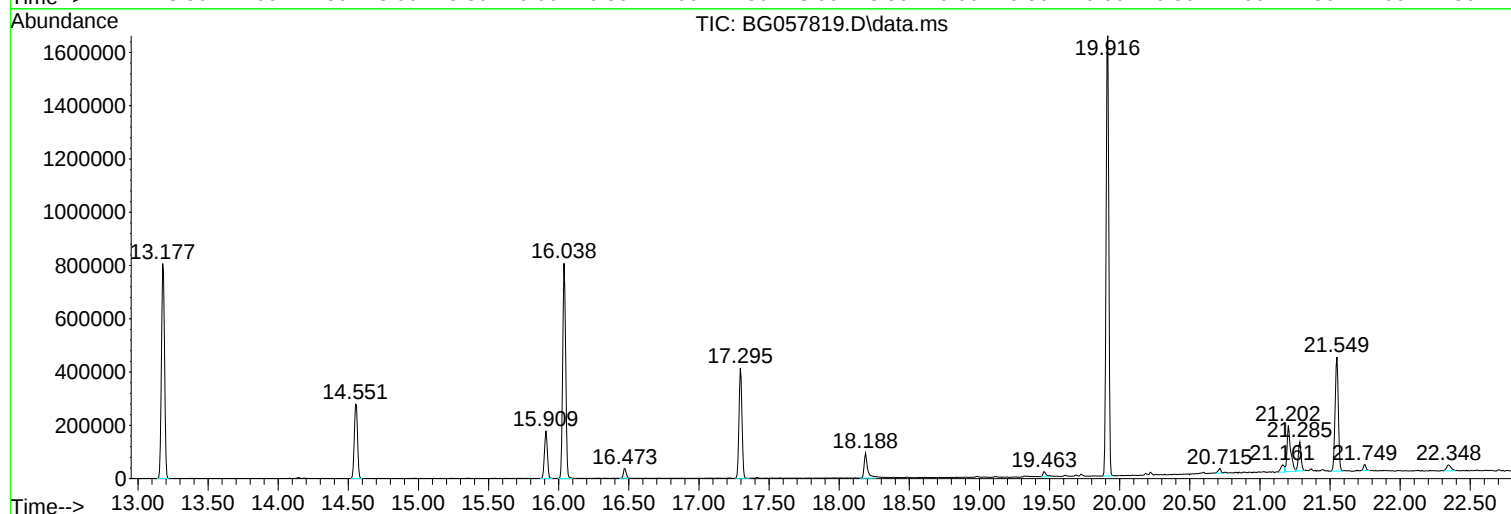
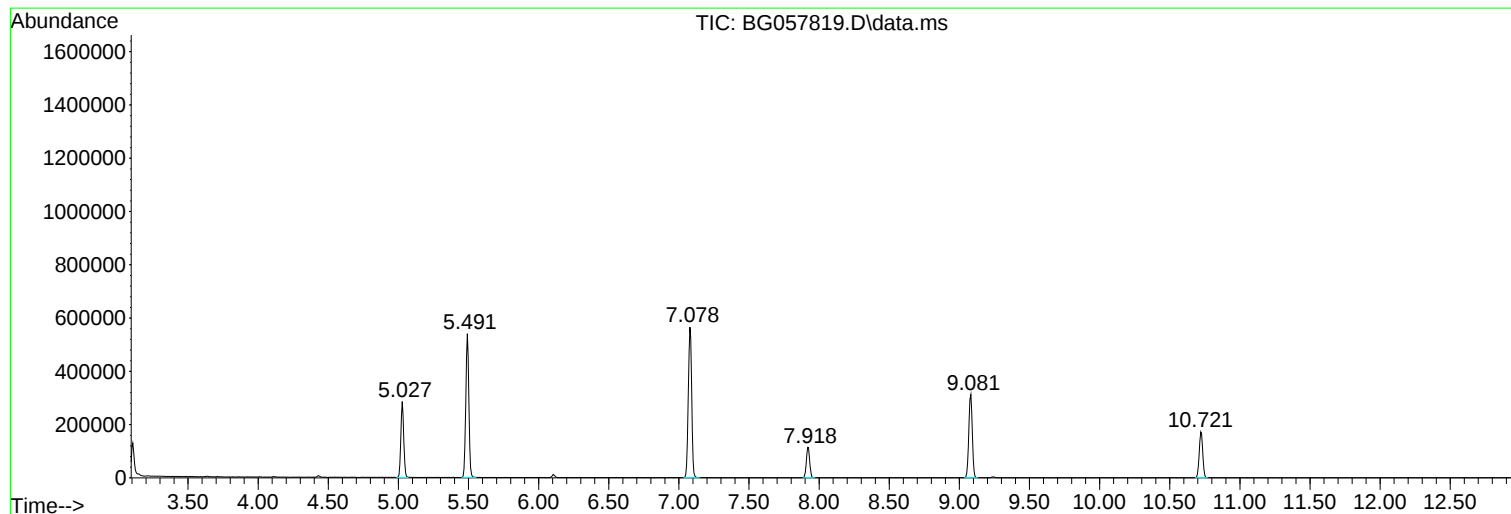
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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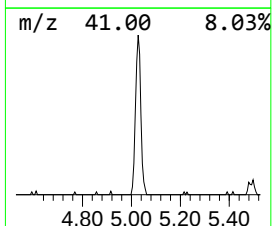
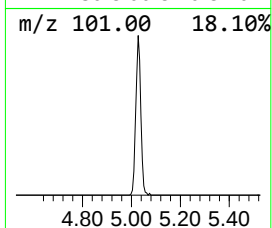
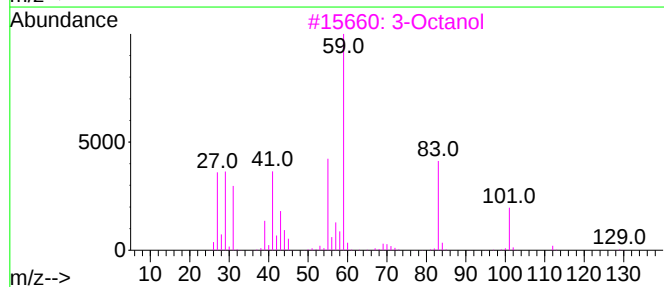
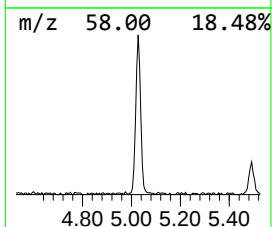
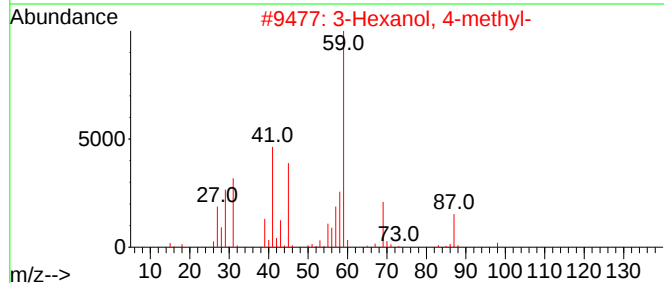
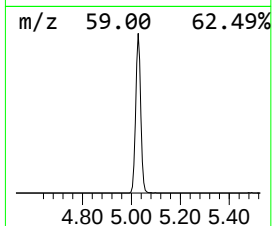
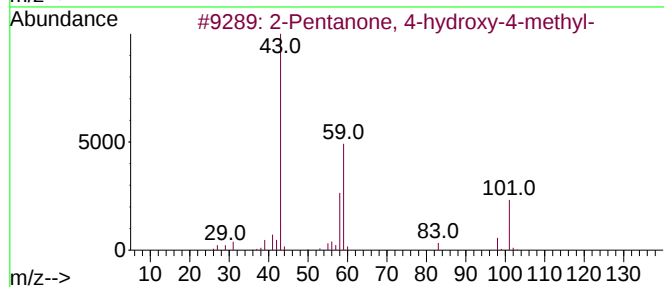
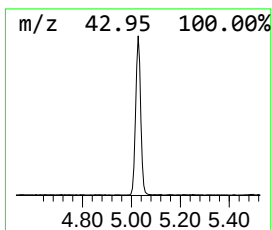
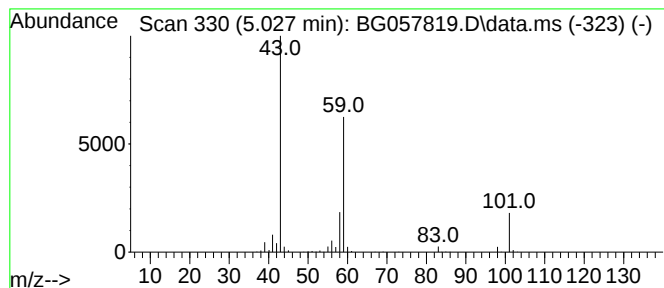
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.027	42.93 ng	409873	1,4-Dichlorobenzene-d4	7.918

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59	
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33	
3	3-Octanol	130	C8H18O	000589-98-0	33	
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33	
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23	



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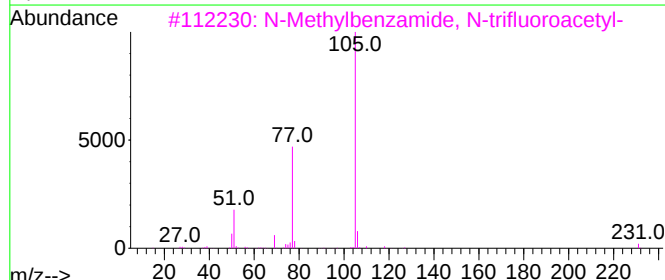
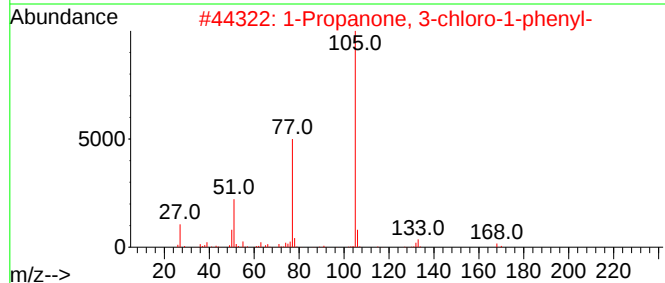
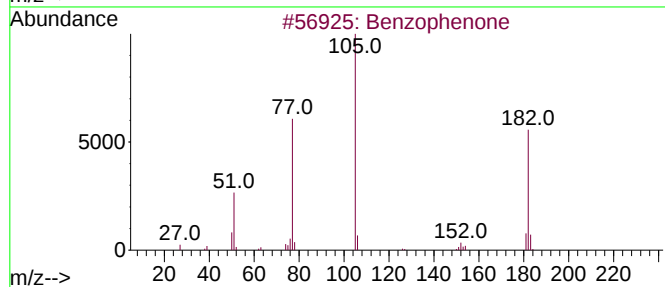
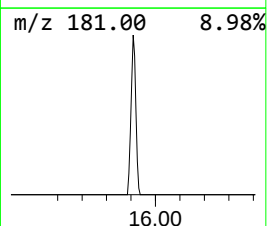
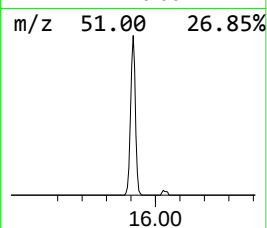
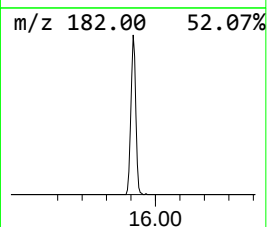
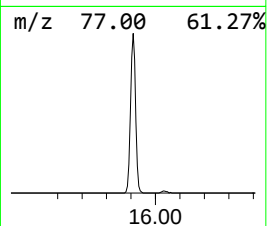
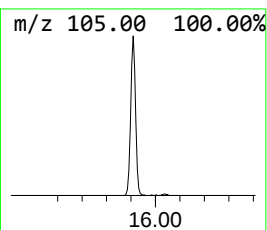
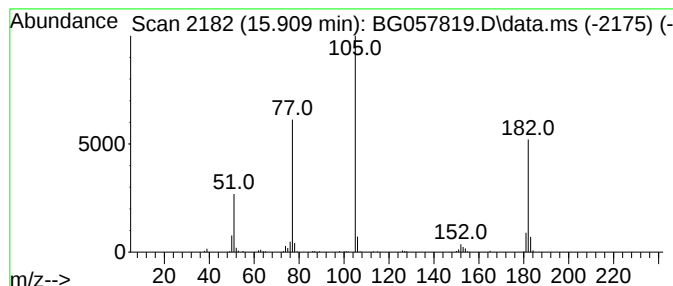
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Peak Number 2 Benzophenone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.909	11.20 ng	247989	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
3			N-Methylbenzamide, N-trifluoroac...	231	C10H8F3NO2	1000446-91-5	47
4			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	47
5			5-Oxo-5-phenylpentanenitrile	173	C11H11NO	1000486-83-7	47



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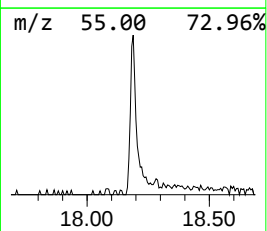
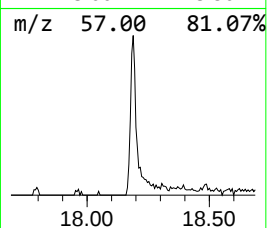
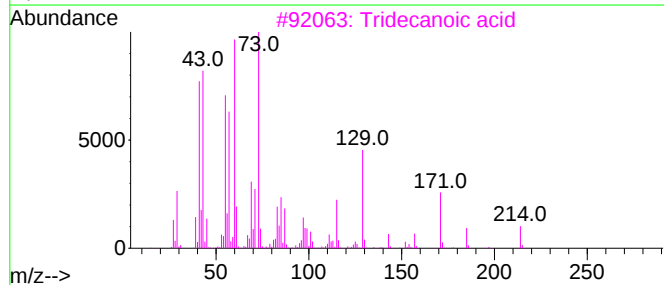
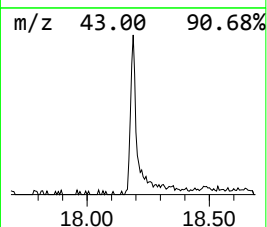
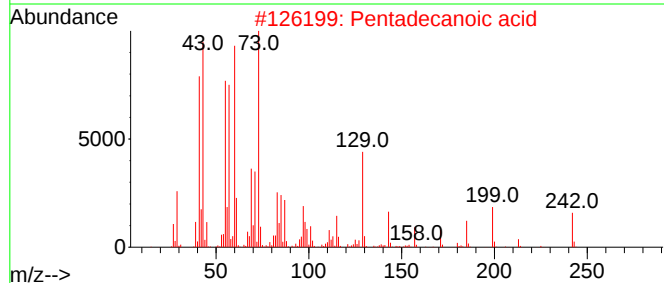
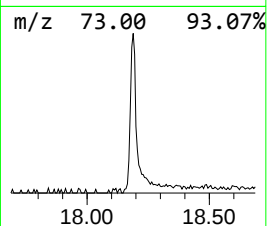
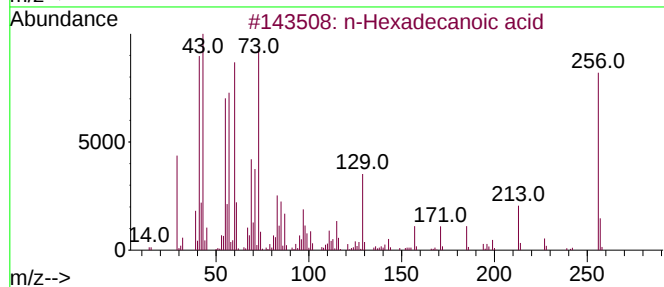
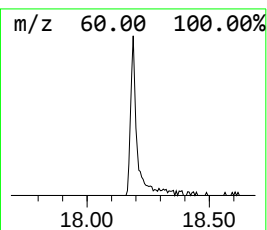
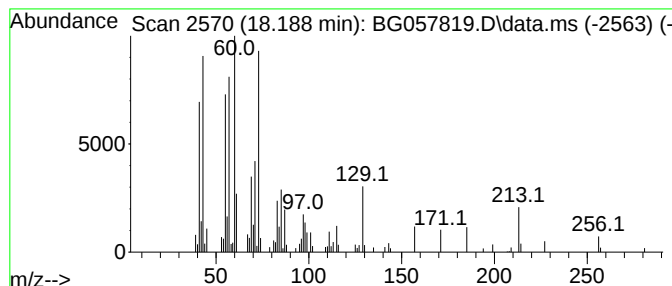
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.188	5.16 ng	159449	Phenanthrene-d10	17.295

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3			Tridecanoic acid	214	C13H26O2	000638-53-9	81
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	25
5			Carbonic acid, octadecyl prop-1-...	354	C22H42O3	1000383-11-5	15



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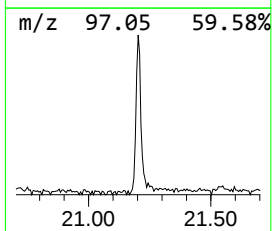
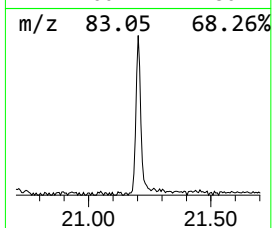
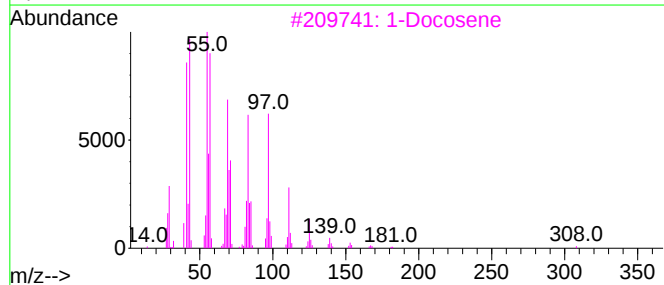
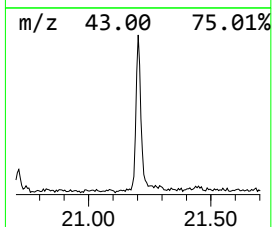
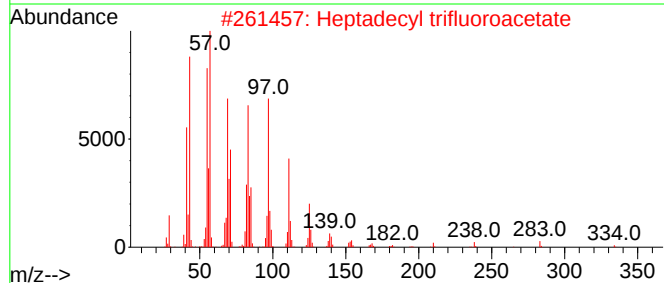
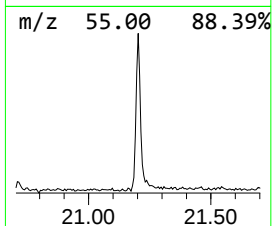
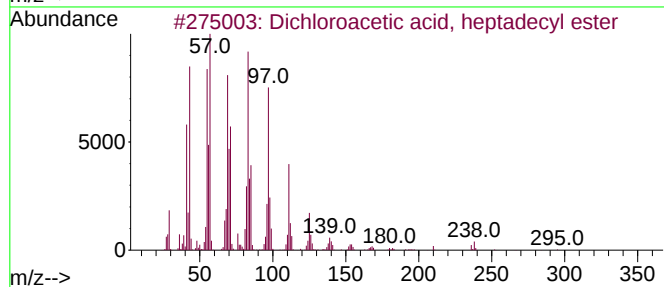
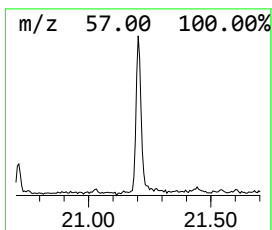
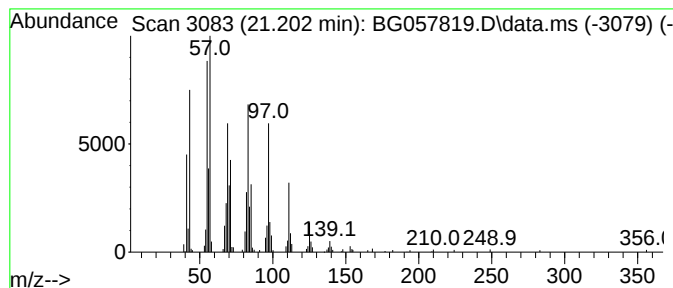
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Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.202	8.79 ng	303583	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
3			1-Docosene	308	C22H44	001599-67-3	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			Octacosanol	410	C28H58O	000557-61-9	91



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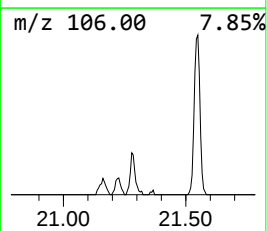
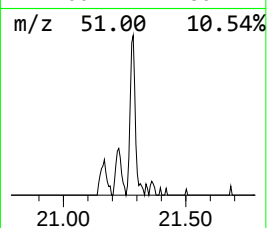
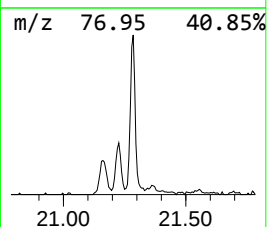
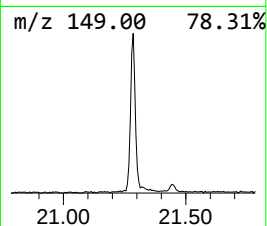
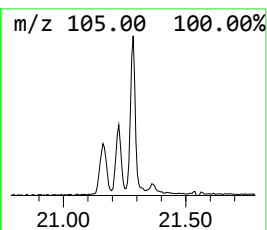
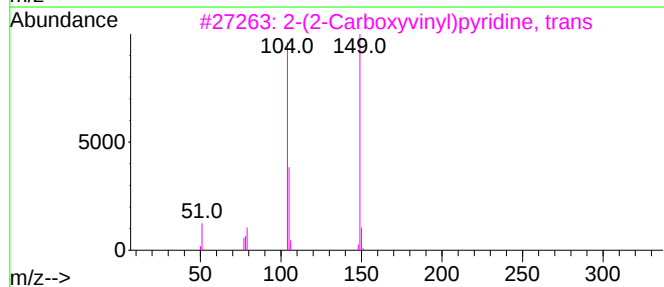
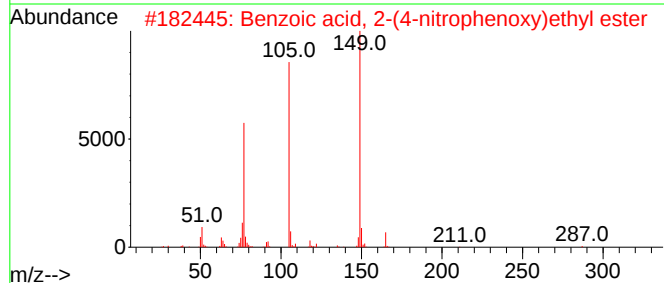
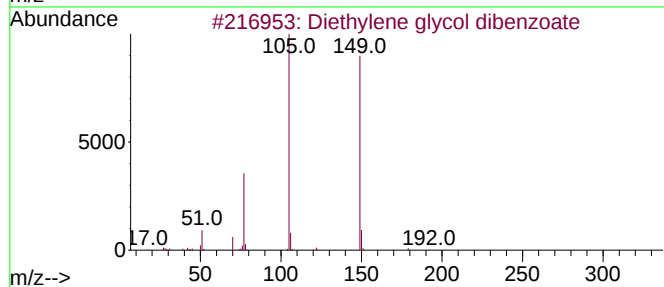
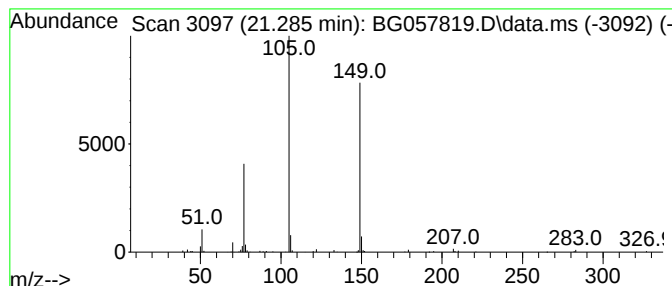
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Diethylene glycol dibenzoate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.285	4.30 ng	148408	Chrysene-d12	21.549

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diethylene glycol dibenzoate	314	C18H18O5	000120-55-8	90
2			Benzoic acid, 2-(4-nitrophenoxy)...	287	C15H13NO5	1000368-92-7	72
3			2-(2-Carboxyvinyl)pyridine, trans	149	C8H7NO2	007340-22-9	52
4			.beta.-Phenylpropiofenone	210	C15H14O	001083-30-3	38
5			Benzeneacetic acid, .alpha.-oxo-...	178	C10H10O3	001603-79-8	35



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.027	42.9	ng	409873	1	7.918	190940	20.0
Benzophenone	15.909	11.2	ng	247989	3	14.557	442923	20.0
n-Hexadecanoic ...	18.188	5.2	ng	159449	4	17.295	618285	20.0
Dichloroacetic ...	21.202	8.8	ng	303583	5	21.549	690728	20.0
Diethylene glyc...	21.285	4.3	ng	148408	5	21.549	690728	20.0