

Data Path : Z:\svoasrv\HPCHEM1\BNA_G\Data\BG062323\
 Data File : BG057842.D
 Acq On : 23 Jun 2023 14:43
 Operator : CG/JU
 Sample : 03337-19
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 WC-11

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: BG057842.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.028	324	330	337	rVB	80958	116200	5.63%	1.071%
2	5.492	402	409	419	rBV	499492	752544	36.46%	6.938%
3	7.084	672	680	691	rBV	512510	866590	41.99%	7.990%
4	7.918	814	822	829	rBV	125575	206448	10.00%	1.903%
5	9.082	1012	1020	1030	rBV	300140	505431	24.49%	4.660%
6	10.727	1292	1300	1307	rBV	191849	336159	16.29%	3.099%
7	13.183	1711	1718	1727	rBV	798896	1235612	59.86%	11.392%
8	14.558	1944	1952	1961	rVB	356608	543778	26.35%	5.013%
9	15.915	2175	2183	2189	rVB	74956	110851	5.37%	1.022%
10	16.044	2198	2205	2215	rBV	768119	1163010	56.35%	10.722%
11	17.301	2412	2419	2426	rBV	488317	717137	34.74%	6.612%
12	18.189	2563	2570	2582	rBV2	100556	159675	7.74%	1.472%
13	19.464	2783	2787	2796	rBV3	23558	39517	1.91%	0.364%
14	19.916	2858	2864	2871	rVB	1614598	2064032	100.00%	19.029%
15	20.221	2913	2916	2921	rVB2	17885	23228	1.13%	0.214%
16	20.715	2996	3000	3004	rVB2	24231	28481	1.38%	0.263%
17	21.209	3079	3084	3094	rBV2	125124	195026	9.45%	1.798%
18	21.285	3095	3097	3107	rVB	15621	23970	1.16%	0.221%
19	21.555	3136	3143	3150	rBV	457315	741496	35.92%	6.836%
20	21.749	3172	3176	3180	rBV	27029	34755	1.68%	0.320%
21	22.348	3274	3278	3285	rVB3	22325	42941	2.08%	0.396%
22	22.713	3335	3340	3346	rVB7	14157	28819	1.40%	0.266%
23	23.018	3386	3392	3398	rVB6	19159	47279	2.29%	0.436%
24	24.704	3669	3679	3693	rBV	301111	863615	41.84%	7.962%

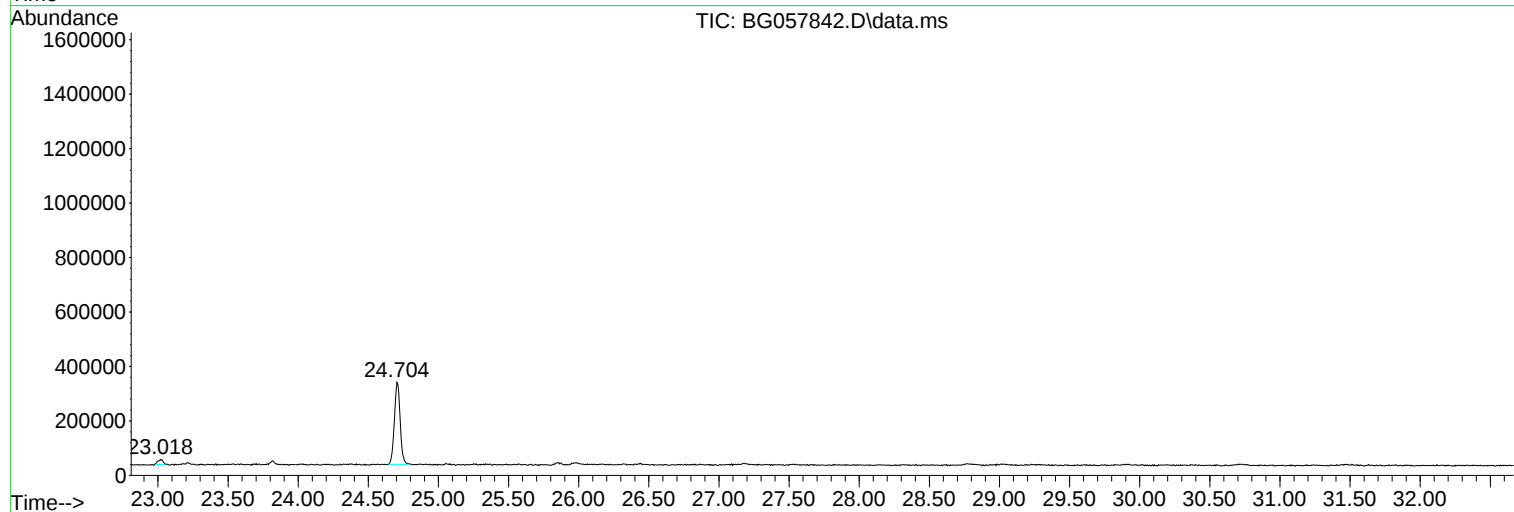
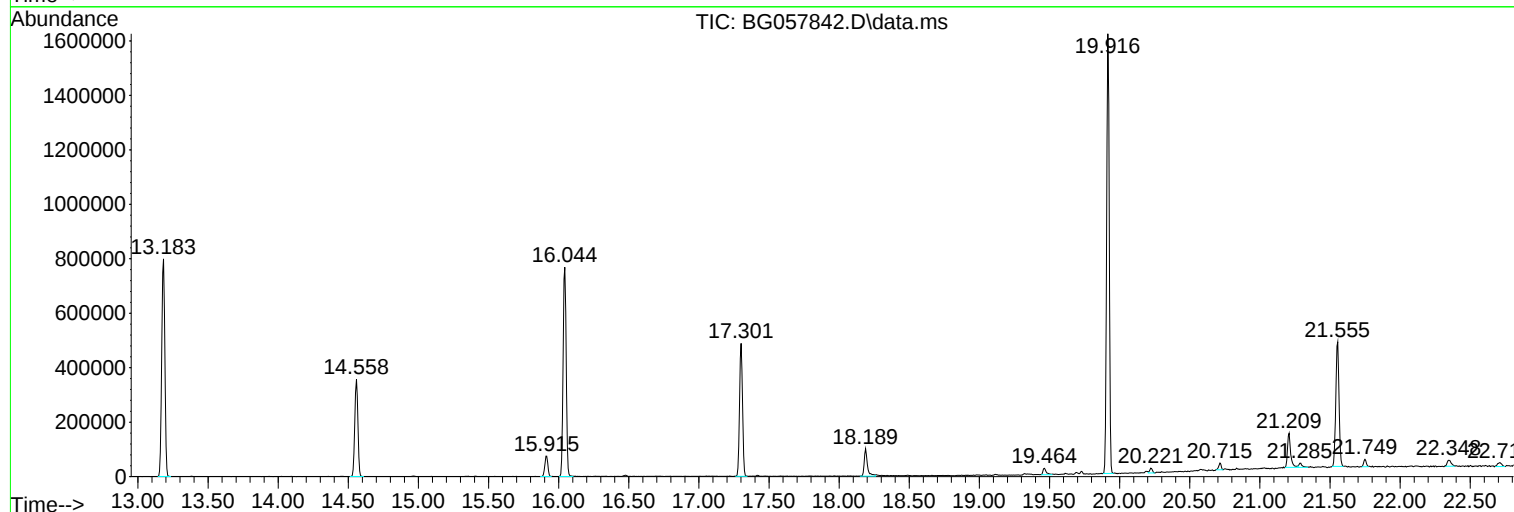
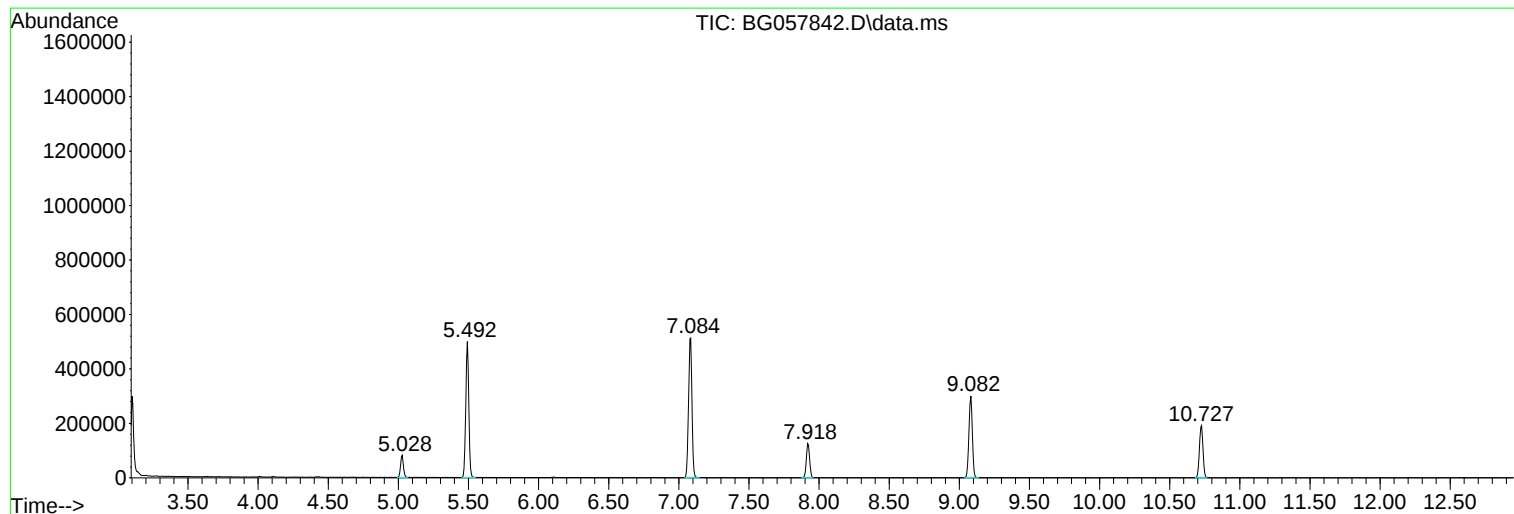
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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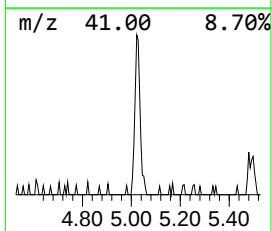
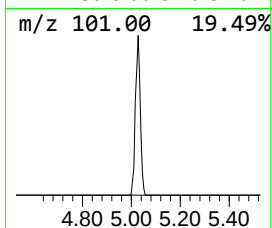
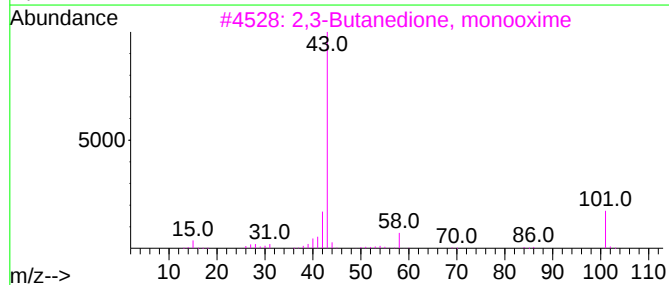
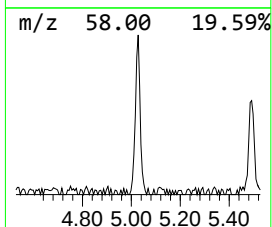
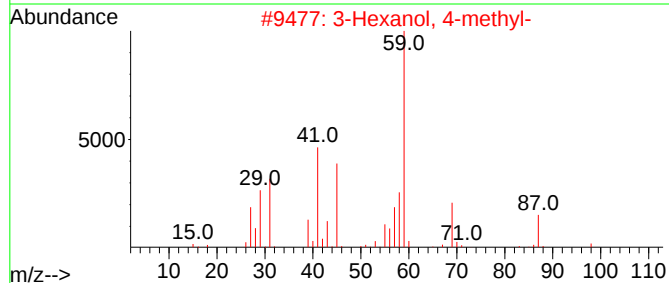
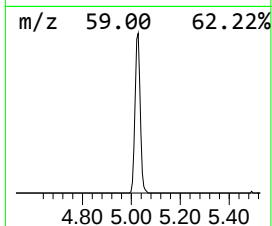
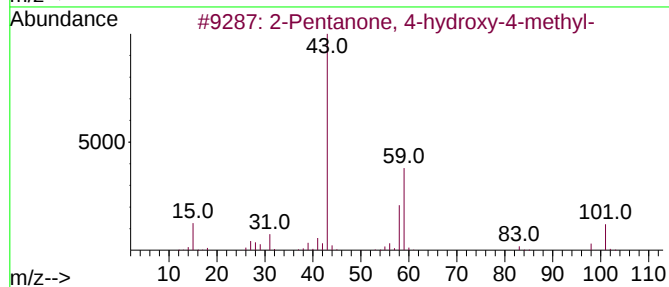
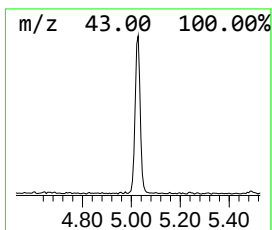
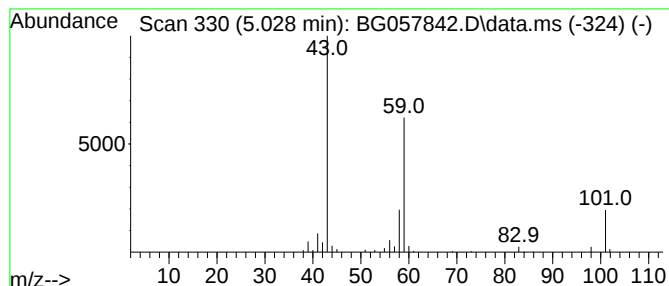
Quant Method : Z:\svoasrv\HPCHEM1\BNA_G\Methods\8270-BG061923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	11.26 ng	116200	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	28	
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16	
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12	
5	Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	12	



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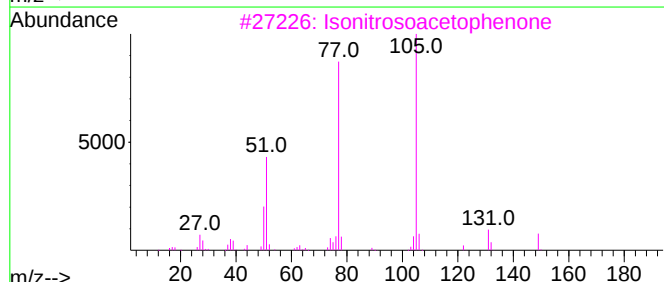
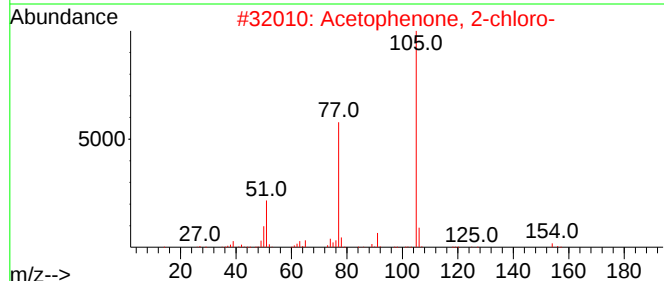
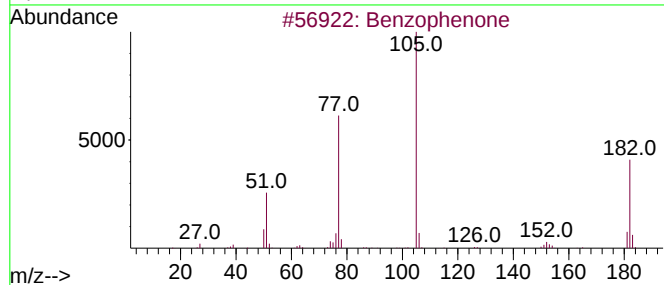
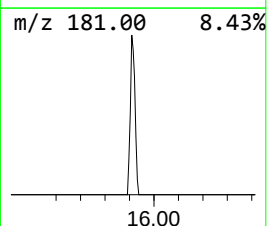
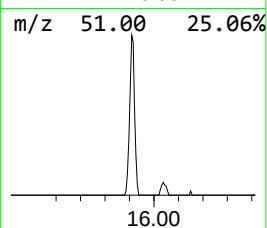
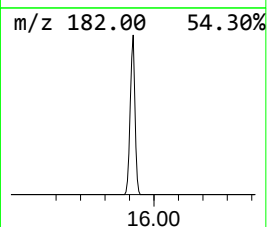
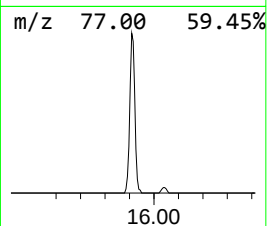
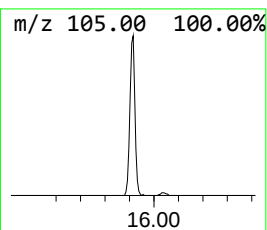
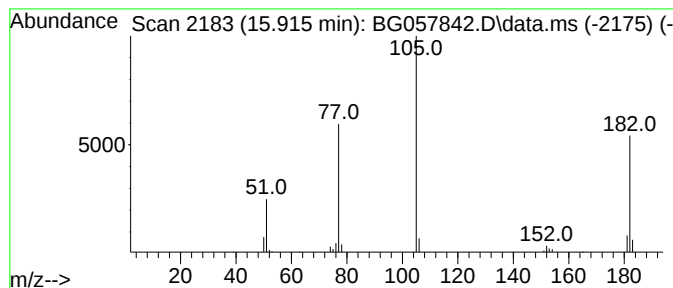
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Peak Number 2 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.915	4.08 ng	110851	Acenaphthene-d10	14.557

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3			Isonitrosoacetophenone	149	C8H7NO2	000532-54-7	47
4			1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47
5			acetic acid, 2-bromo-, 2-oxo-2-p...	256	C10H9BrO3	1000401-50-0	47



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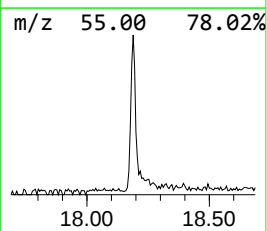
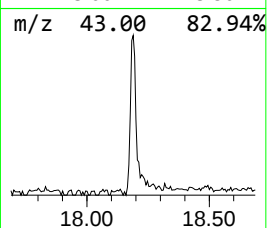
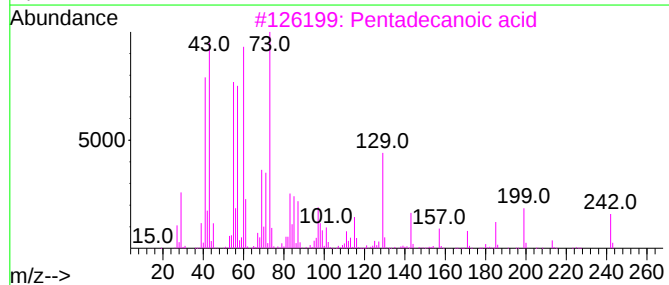
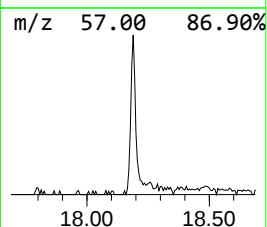
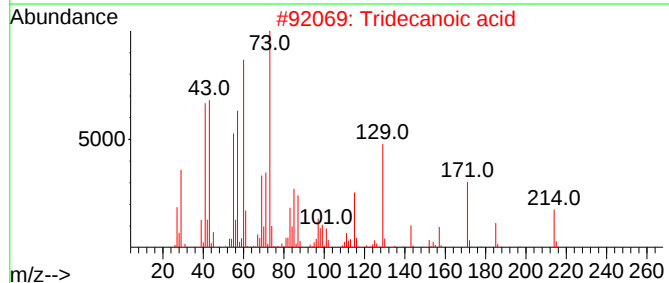
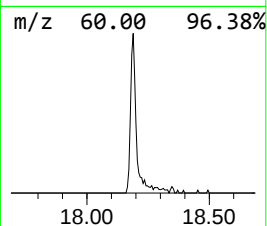
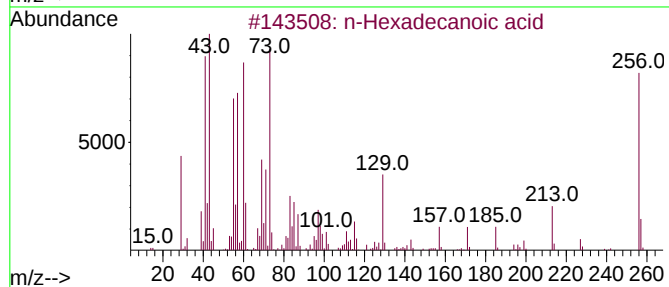
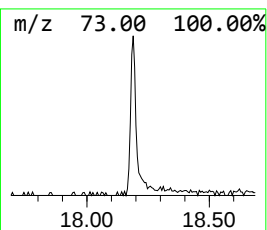
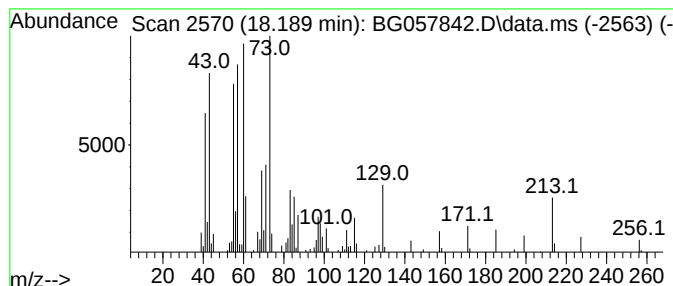
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.189	4.45 ng	159675	Phenanthrene-d10	17.301

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tridecanoic acid	214	C13H26O2	000638-53-9	95
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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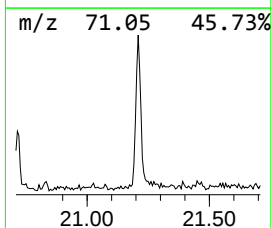
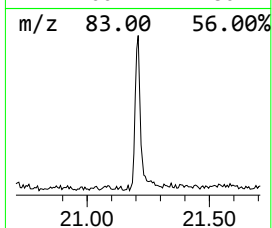
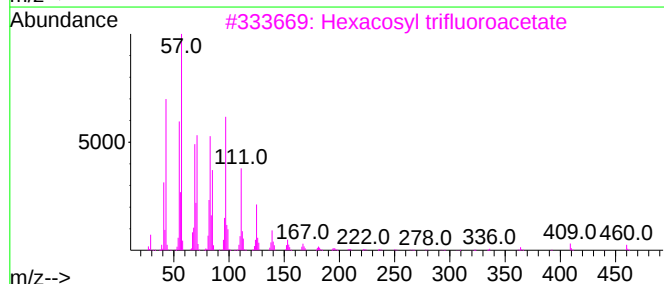
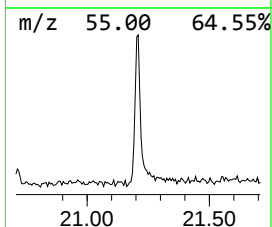
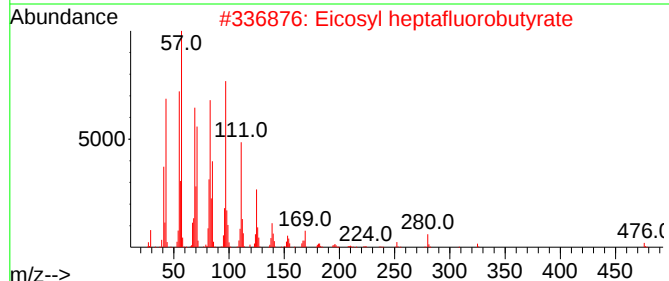
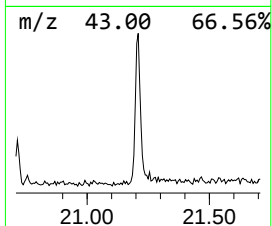
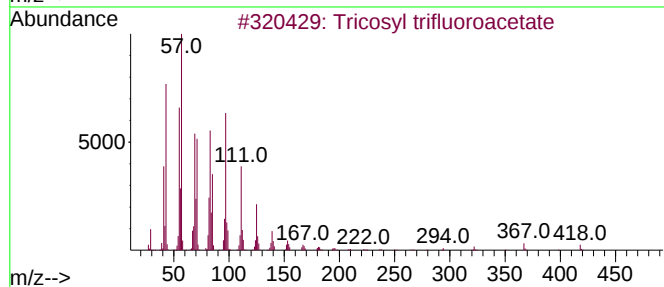
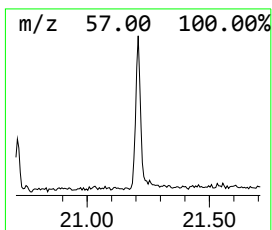
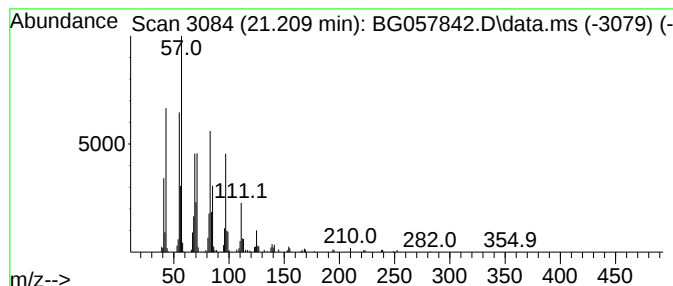
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Peak Number 4 Tricosyl trifluoroacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.209	5.26 ng	195026	Chrysene-d12	21.555

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tricosyl trifluoroacetate	436	C25H47F3O2	1000351-75-1	91
2			Eicosyl heptafluorobutyrate	494	C24H41F7O2	1000351-83-5	91
3			Hexacosyl trifluoroacetate	478	C28H53F3O2	1000351-75-0	91
4			Heptafluorobutyric acid, n-octad...	466	C22H37F7O2	000400-57-7	91
5			Hexacosyl heptafluorobutyrate	578	C30H53F7O2	1000351-83-3	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.028	11.3	ng	116200	1	7.918	206448	20.0
Benzophenone	15.915	4.1	ng	110851	3	14.557	543778	20.0
n-Hexadecanoic ...	18.189	4.5	ng	159675	4	17.301	717137	20.0
Tricosyl triflu...	21.209	5.3	ng	195026	5	21.555	741496	20.0