

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM031021\
 Data File : BM029079.D
 Acq On : 10 Mar 2021 20:49
 Operator : CG/JU
 Sample : M1613-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 S-1

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-BM022321.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029079.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	377	382	396	rBV	136400	194922	49.82%	9.642%
2	6.857	649	658	675	rBV	124008	203972	52.13%	10.090%
3	7.663	790	795	802	rBB	27969	41177	10.52%	2.037%
4	8.839	989	995	1006	rBB	77113	124604	31.85%	6.164%
5	10.457	1264	1270	1279	rBB	34560	55717	14.24%	2.756%
6	12.945	1687	1693	1700	rBV	173766	246591	63.02%	12.198%
7	13.798	1834	1838	1844	rBB	6479	7934	2.03%	0.392%
8	14.333	1924	1929	1935	rBB2	49937	69841	17.85%	3.455%
9	15.833	2178	2184	2196	rBB	139135	191273	48.88%	9.462%
10	17.080	2390	2396	2402	rBV	60252	80262	20.51%	3.970%
11	17.974	2543	2548	2557	rBV	29655	40740	10.41%	2.015%
12	18.445	2623	2628	2634	rVB	2151	3964	1.01%	0.196%
13	18.709	2669	2673	2679	rVB	14592	18016	4.60%	0.891%
14	19.127	2738	2744	2748	rBV2	4716	8176	2.09%	0.404%
15	19.256	2762	2766	2775	rBV2	34748	45717	11.68%	2.261%
16	19.703	2837	2842	2848	rBV	333080	391279	100.00%	19.356%
17	20.568	2986	2989	2995	rVB2	3960	4737	1.21%	0.234%
18	20.980	3054	3059	3066	rBV2	33504	50952	13.02%	2.520%
19	21.250	3101	3105	3111	rBV	87571	113902	29.11%	5.634%
20	22.062	3241	3243	3247	rBV5	6340	6654	1.70%	0.329%
21	23.409	3466	3472	3481	rBV	69677	121106	30.95%	5.991%

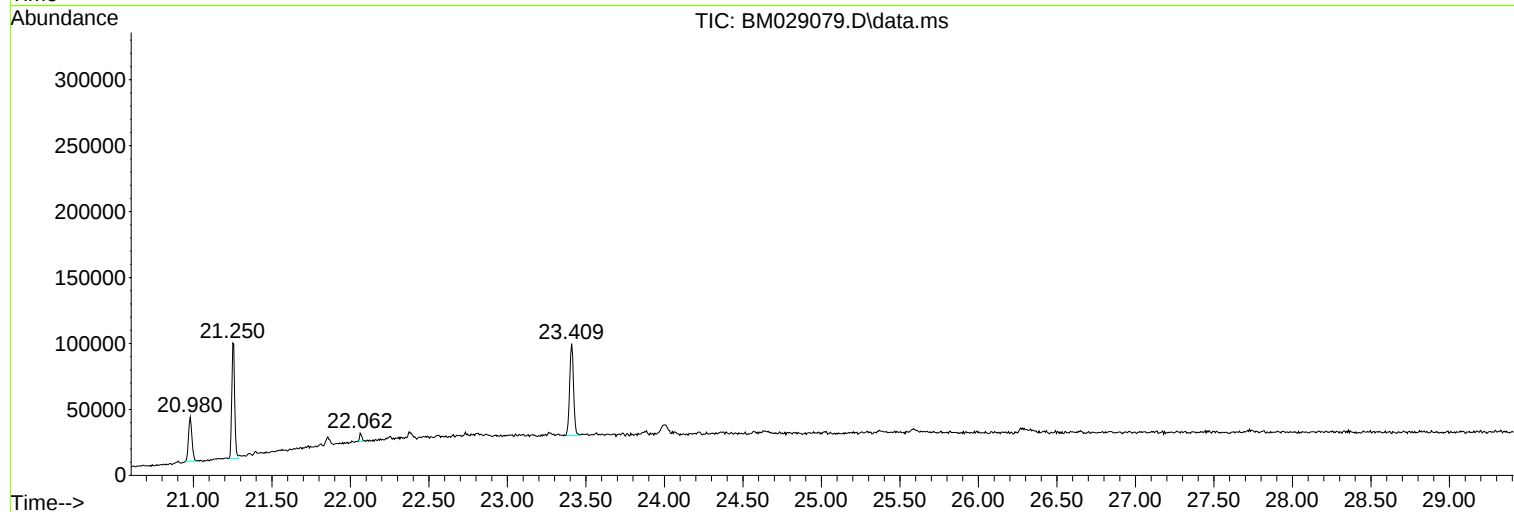
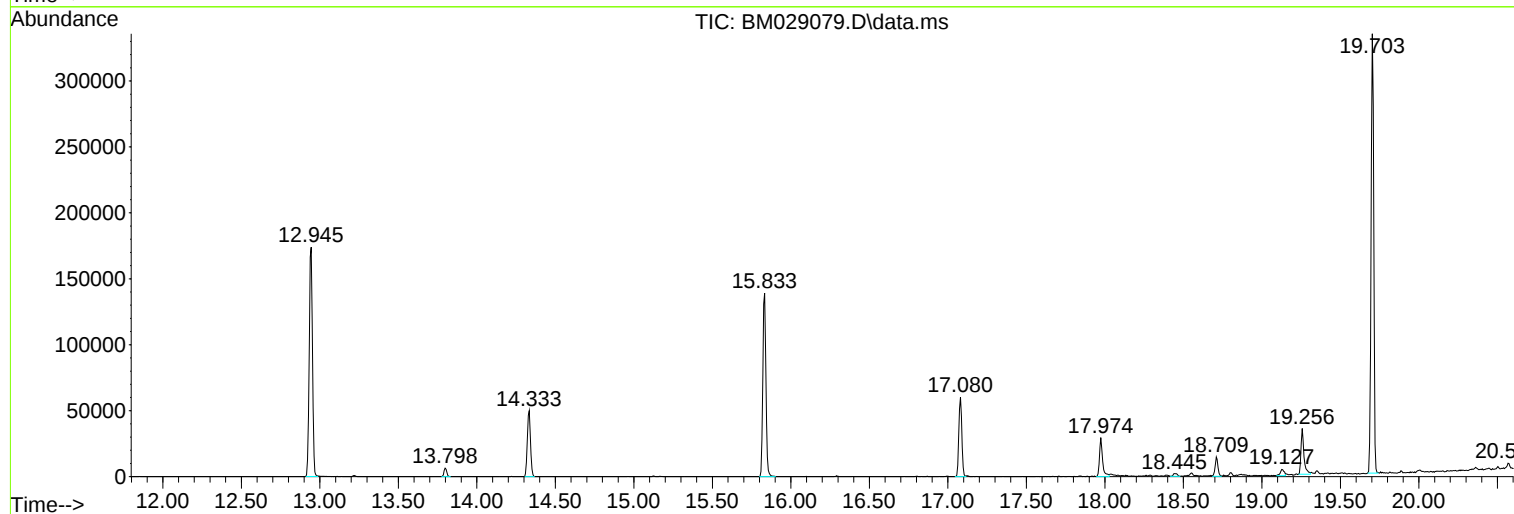
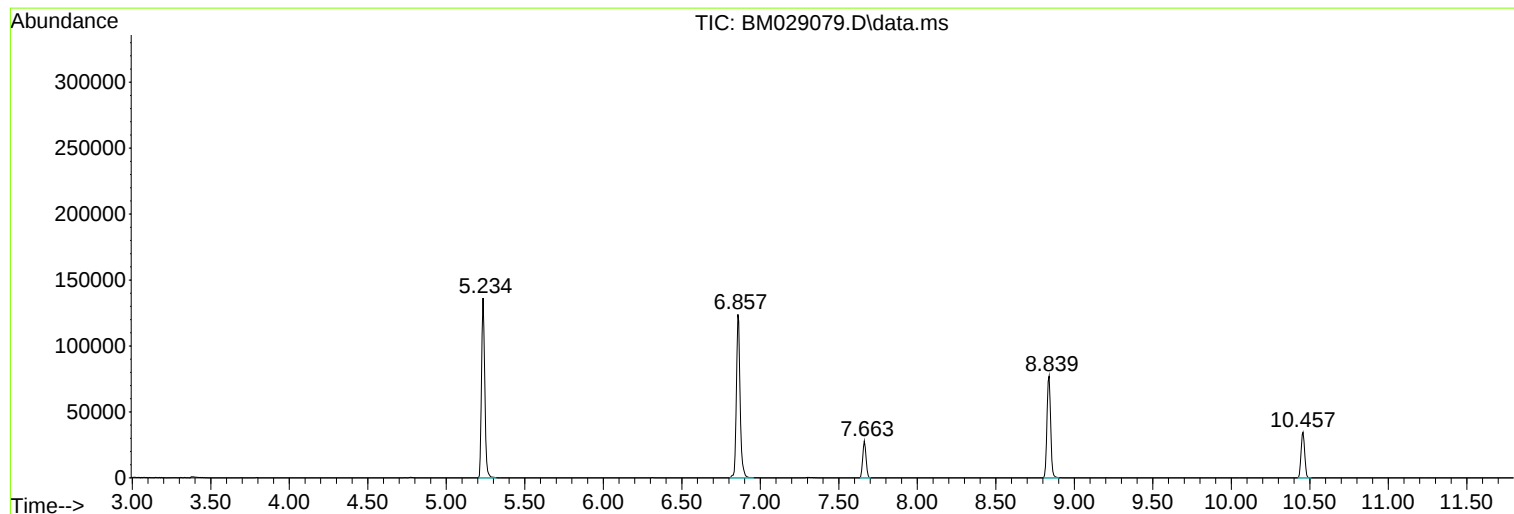
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : CG/JU
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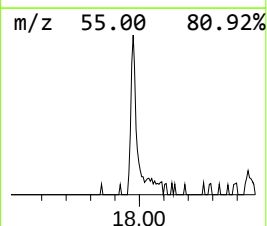
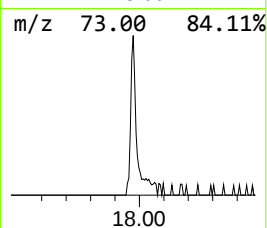
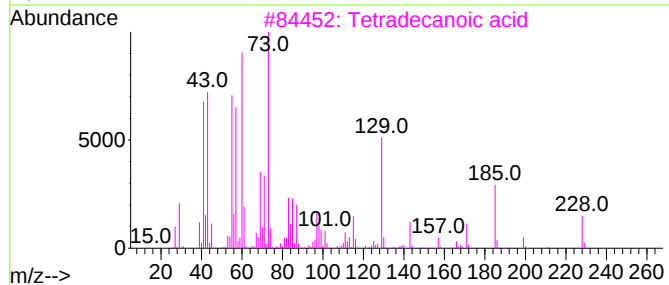
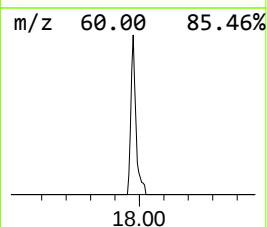
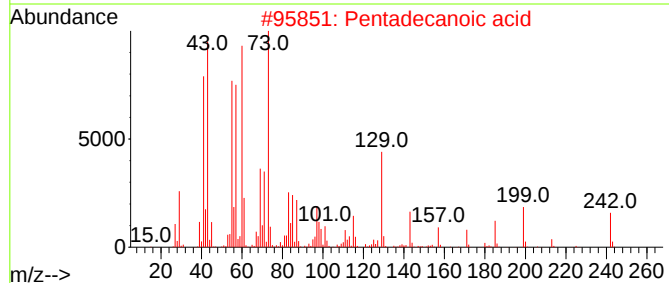
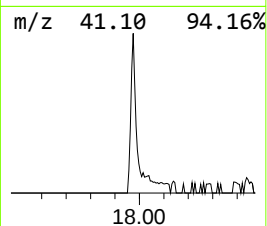
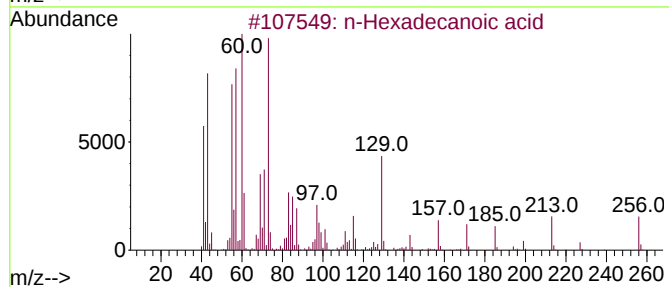
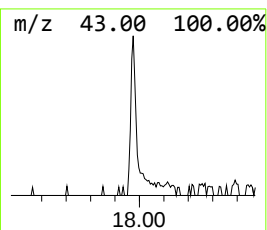
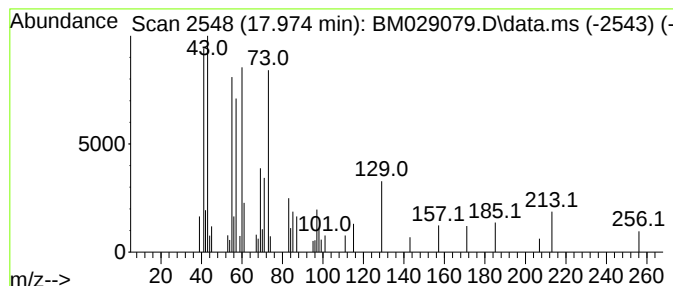
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
17.974	10.15 ng	40740	Phenanthrene-d10	17.080

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	87
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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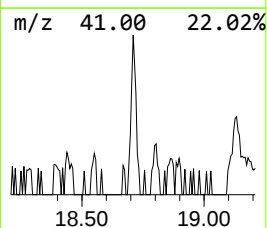
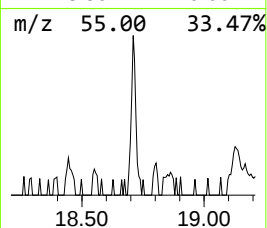
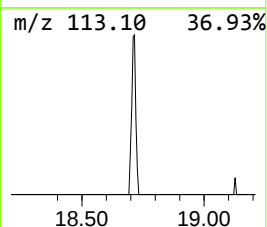
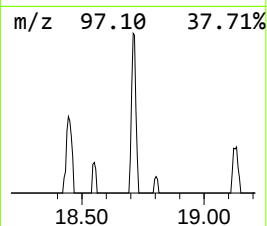
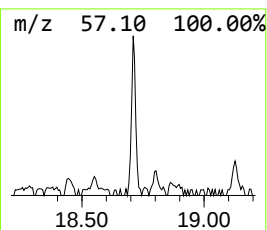
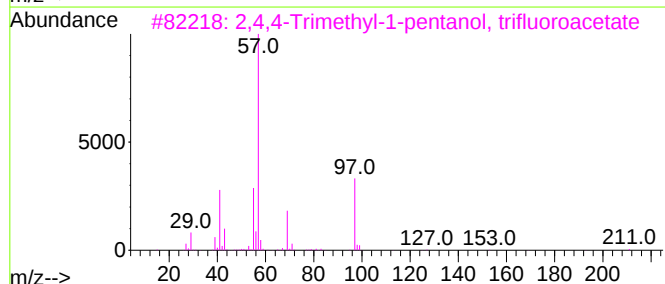
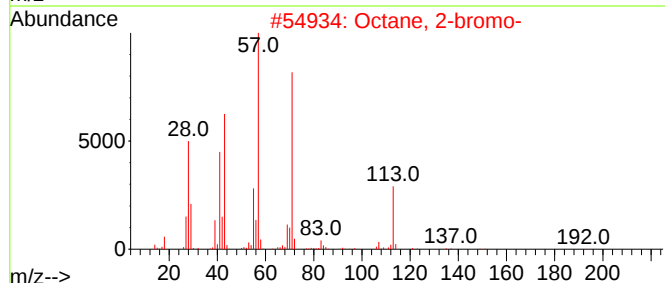
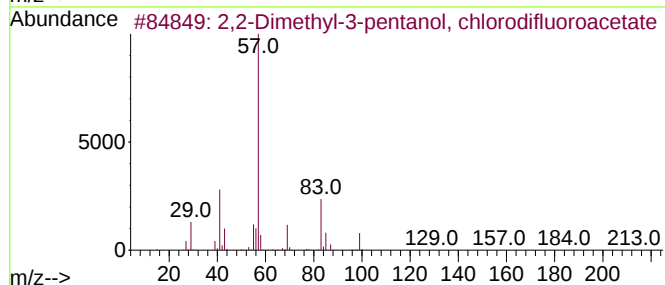
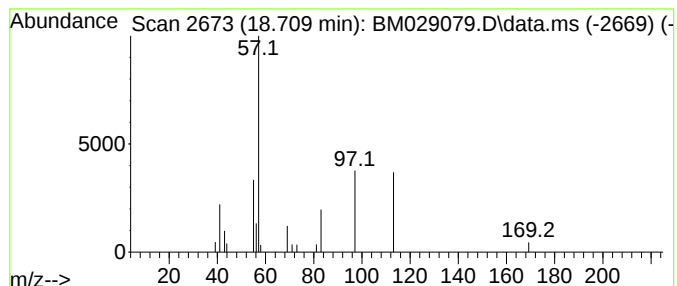
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown18.709 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.709	4.49 ng	18016	Phenanthrene-d10	17.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,2-Dimethyl-3-pentanol, chlorod...	228	C9H15ClF2O2	1000376-26-4	32		
2	Octane, 2-bromo-	192	C8H17Br	000557-35-7	23		
3	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	17		
4	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	12		
5	2,4,4-Trimethyl-1-pentanol, hept...	326	C12H17F7O2	1000365-01-4	12		



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S-1

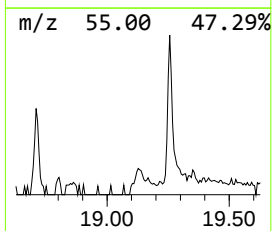
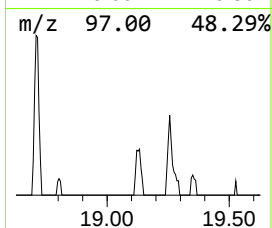
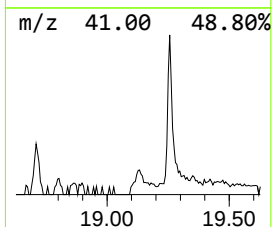
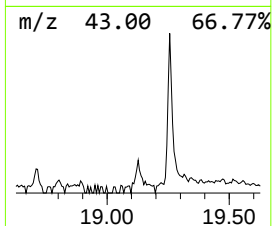
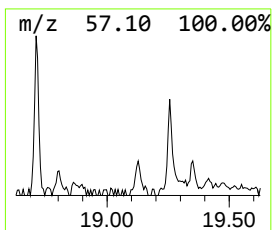
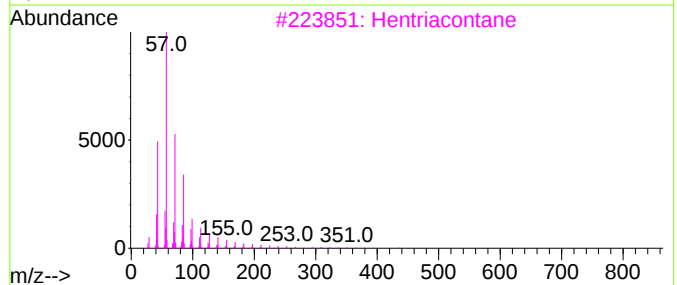
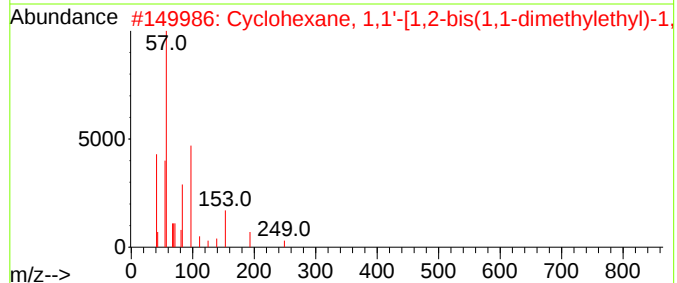
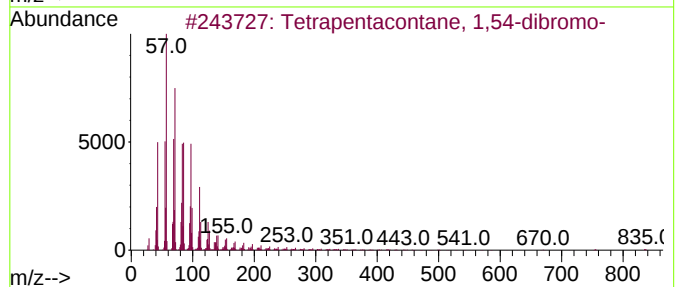
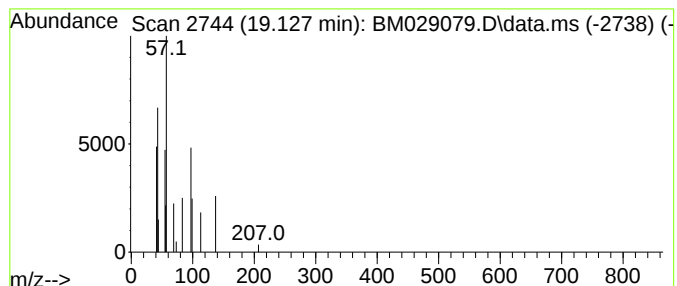
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown19.127 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.127	2.04 ng	8176	Phenanthrene-d10	17.080

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetrapentacontane, 1,54-dibromo-	915	C54H108Br2	1000156-09-4	36
2			Cyclohexane, 1,1'-[1,2-bis(1,1-d...	306	C22H42	065149-85-1	32
3			Hentriacontane	437	C31H64	000630-04-6	23
4			11-Tricosene	322	C23H46	052078-56-5	12
5			Octadecane, 1-bromo-	332	C18H37Br	000112-89-0	12



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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-1

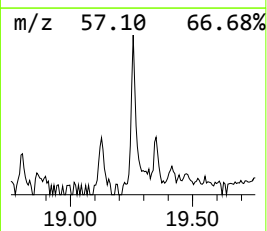
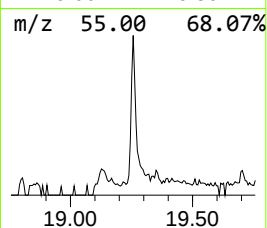
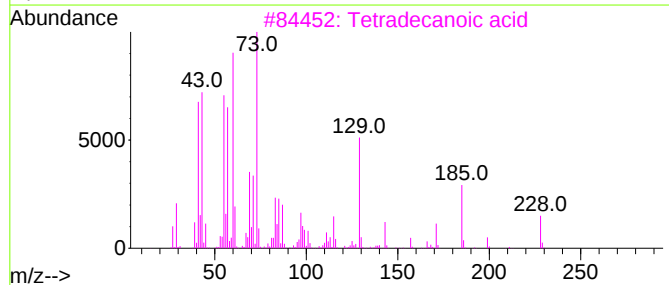
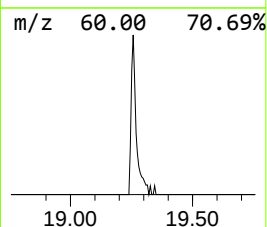
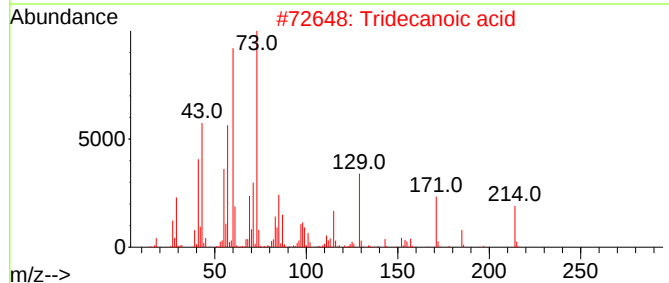
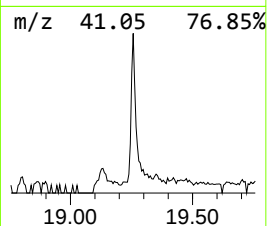
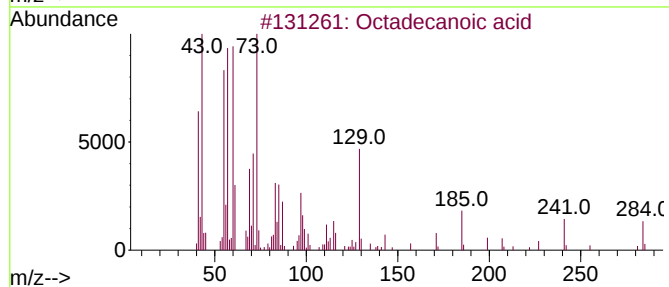
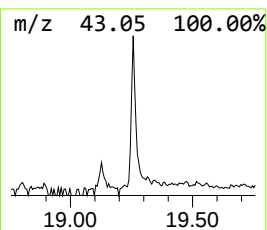
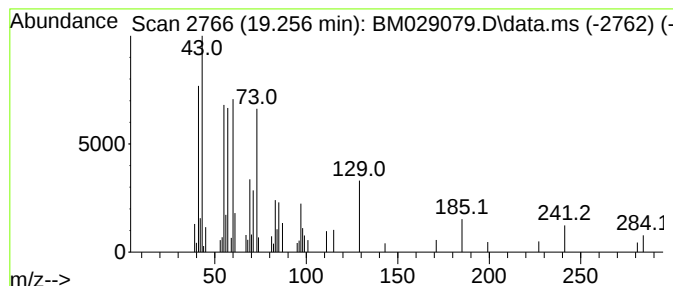
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.256	8.03 ng	45717	Chrysene-d12	21.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	52
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	47
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	43



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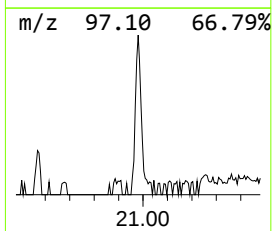
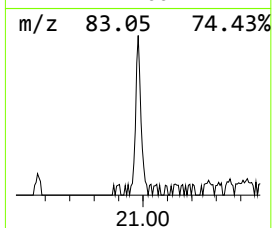
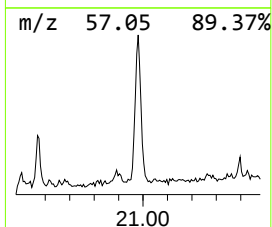
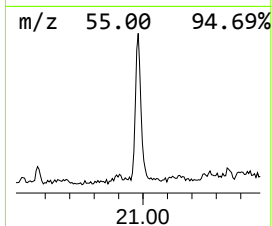
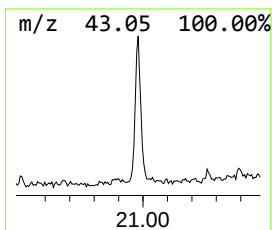
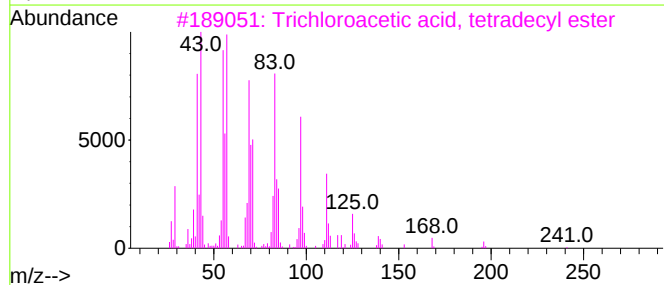
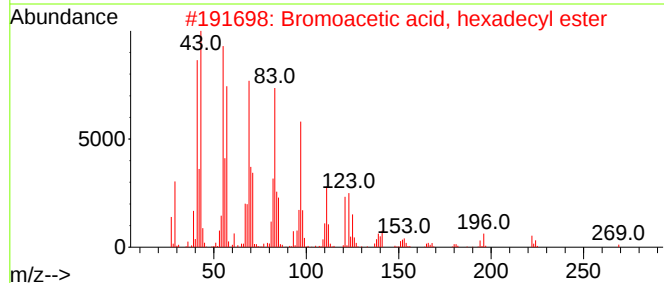
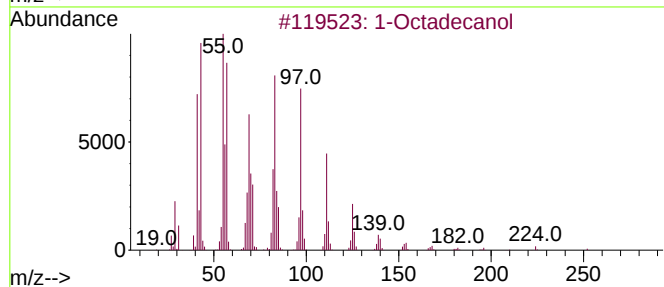
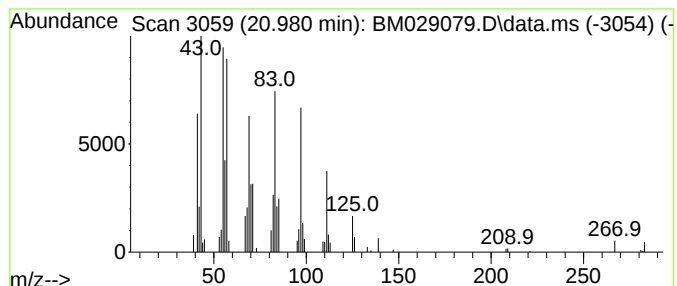
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Octadecanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.980	8.95 ng	50952	Chrysene-d12	21.256

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octadecanol	270	C18H38O	000112-92-5	91
2			Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3			Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4			n-Heptadecanol-1	256	C17H36O	001454-85-9	91
5			1-Heneicosanol	312	C21H44O	015594-90-8	87



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	17.974	10.2	ng	40740	4	17.080	80262	20.0
unknown18.709	18.709	4.5	ng	18016	4	17.080	80262	20.0
unknown19.127	19.127	2.0	ng	8176	4	17.080	80262	20.0
Octadecanoic acid	19.256	8.0	ng	45717	5	21.256	113902	20.0
1-Octadecanol	20.980	8.9	ng	50952	5	21.256	113902	20.0