

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090319\
 Data File : BM022501.D
 Acq On : 03 Sep 2019 14:04
 Operator : HP/JU
 Sample : K4619-15
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 TP5-COMP

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 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-BM082919.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.128	359	364	381	rBB	239731	371643	41.17%	7.593%
2	6.704	626	632	645	rBV	215878	390081	43.22%	7.969%
3	7.039	683	689	701	rBV	284537	446442	49.46%	9.121%
4	7.504	762	768	775	rBB	77184	118464	13.12%	2.420%
5	7.810	815	820	829	rBB	223477	352021	39.00%	7.192%
6	8.681	962	968	991	rBV	112204	241826	26.79%	4.940%
7	10.280	1234	1240	1259	rBV	54464	127566	14.13%	2.606%
8	12.768	1657	1663	1677	rBV	299359	536308	59.42%	10.957%
9	13.668	1811	1816	1825	rBV2	11433	19464	2.16%	0.398%
10	14.174	1896	1902	1913	rBB2	96929	163411	18.10%	3.338%
11	15.686	2154	2159	2178	rBB	251960	450586	49.92%	9.205%
12	16.945	2368	2373	2387	rBV	86426	170411	18.88%	3.481%
13	17.833	2519	2524	2537	rVB2	35252	59426	6.58%	1.214%
14	19.127	2739	2744	2758	rBV2	14605	29880	3.31%	0.610%
15	19.580	2816	2821	2833	rBV	721476	902598	100.00%	18.440%
16	20.850	3032	3037	3042	rBV4	27043	43942	4.87%	0.898%
17	21.162	3085	3090	3100	rBV	130427	211876	23.47%	4.329%
18	22.627	3335	3339	3343	rBV3	17451	25743	2.85%	0.526%
19	23.156	3427	3429	3435	rVB4	15472	21418	2.37%	0.438%
20	23.344	3456	3461	3474	rVB	95359	211726	23.46%	4.326%

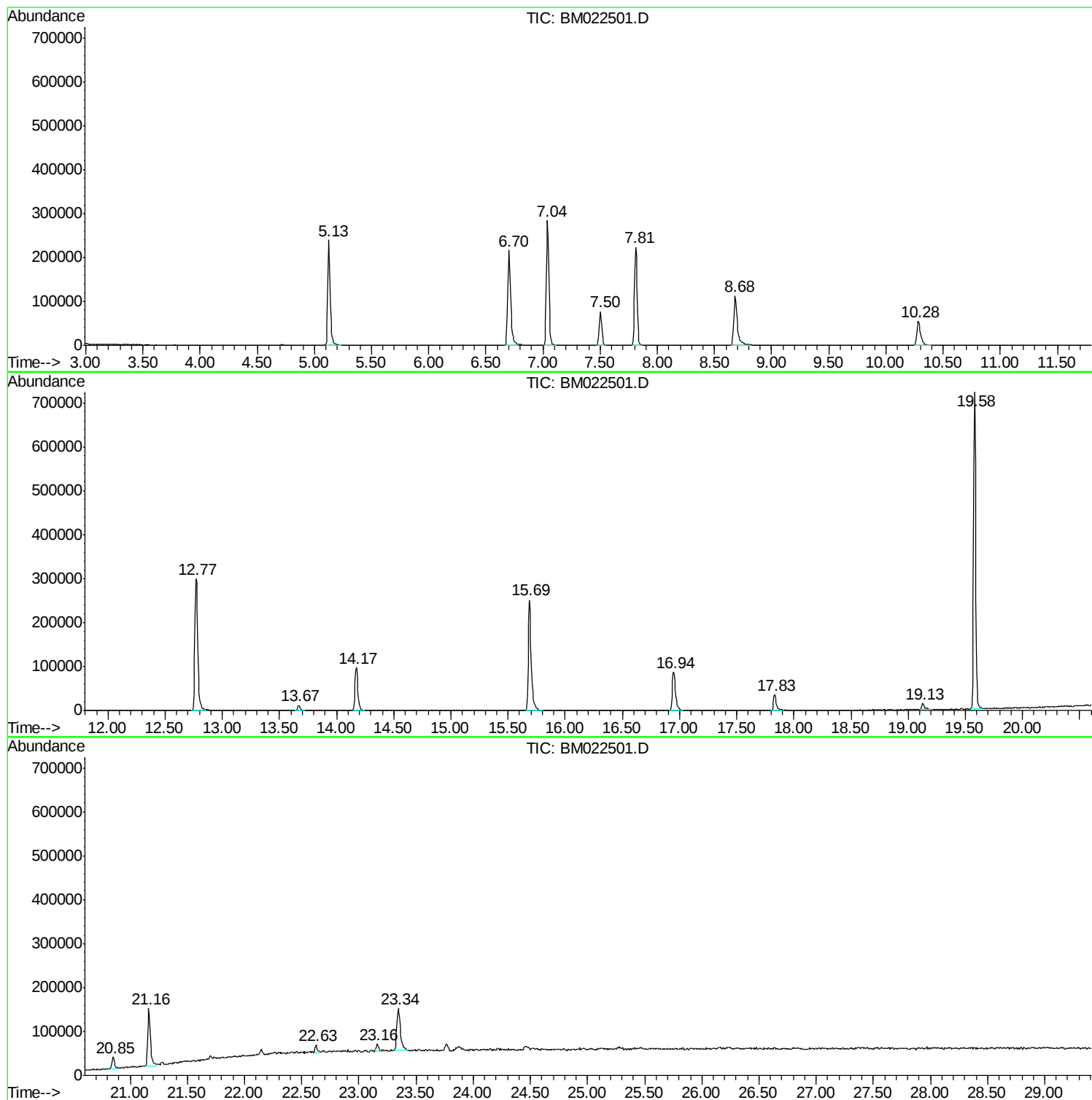
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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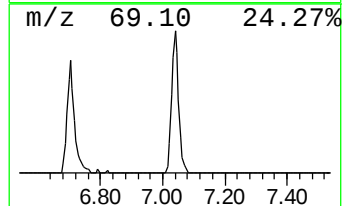
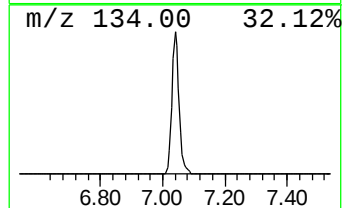
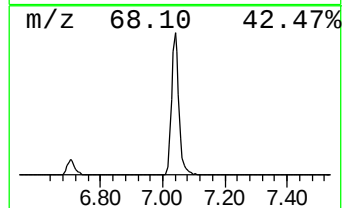
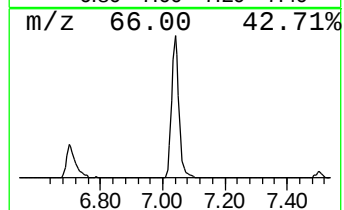
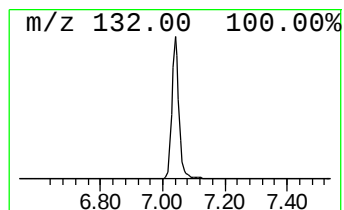
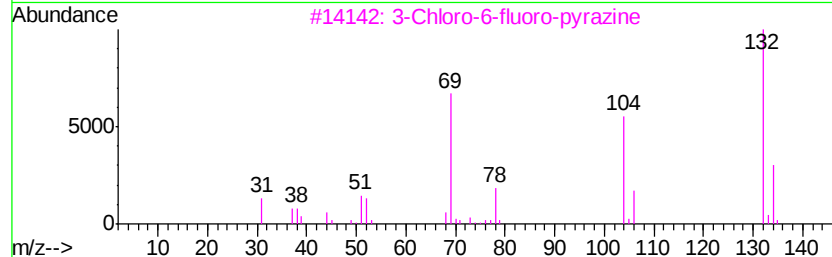
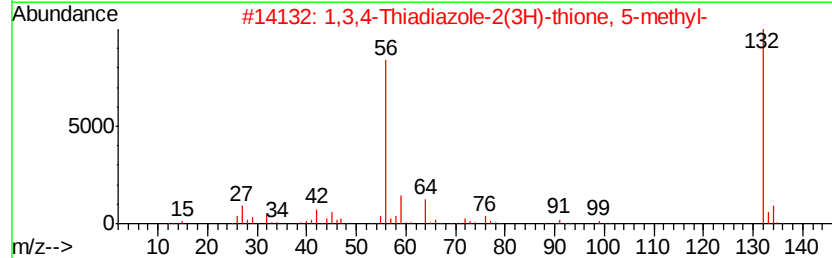
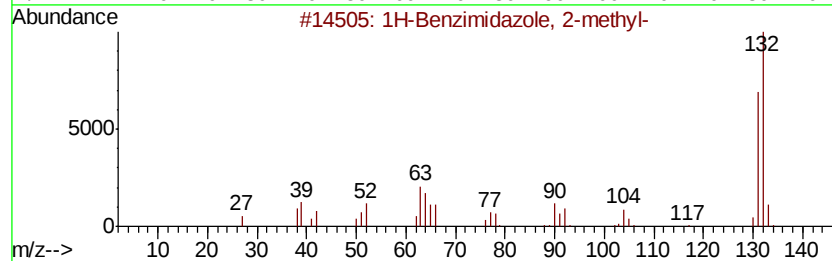
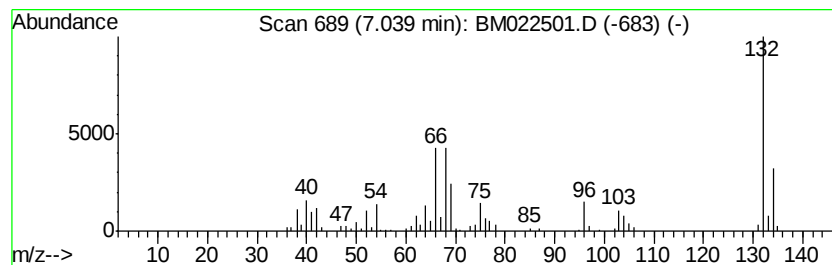
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 1 unknown7.04 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.04	75.37 ng	446442	1,4-Dichlorobenzene-d4	7.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	18
2		1,3,4-Thiadiazole-2(3H)-thione, ...	132	C3H4N2S2	029490-19-5	14
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	14
5		3H-1,2-Dithiol-3-one, 5-methyl-	132	C4H4OS2	003620-08-4	10



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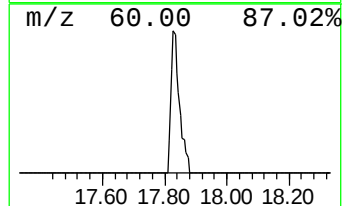
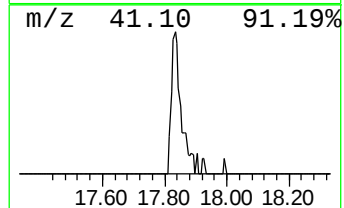
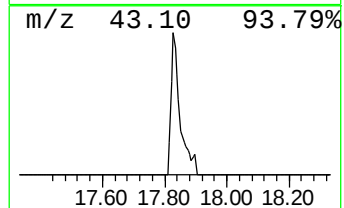
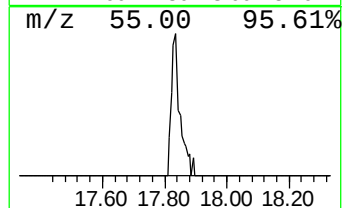
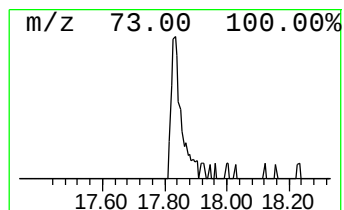
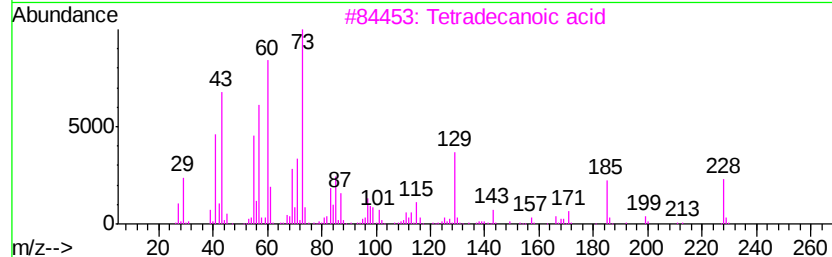
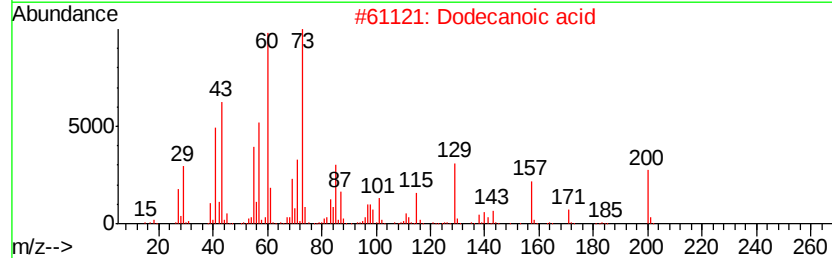
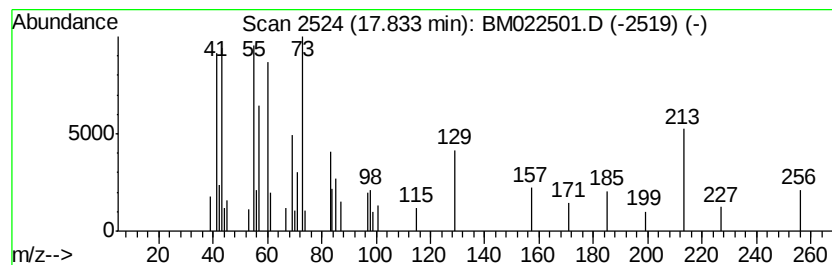
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.83	6.97 ng	59426	Phenanthrene-d10	16.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Dodecanoic acid	200	C12H24O2	000143-07-7	47
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	46
4		Tridecanoic acid	214	C13H26O2	000638-53-9	43
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	43



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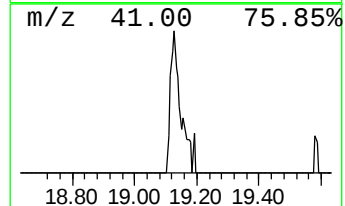
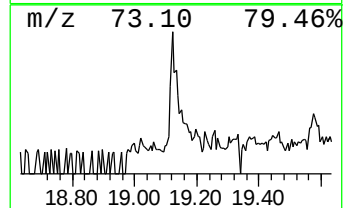
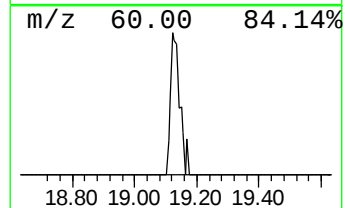
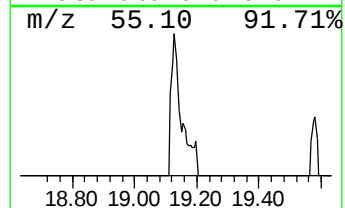
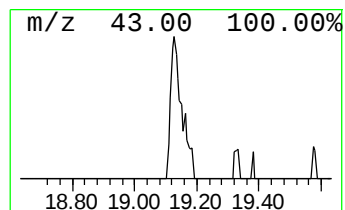
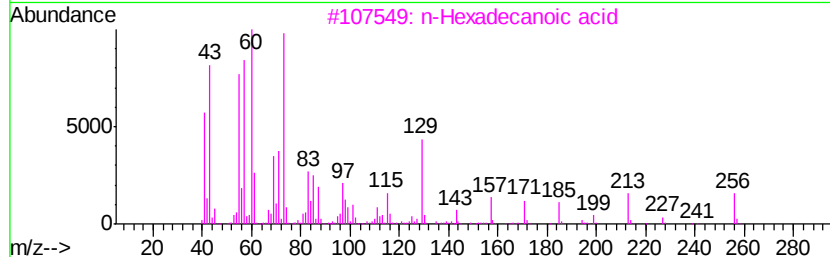
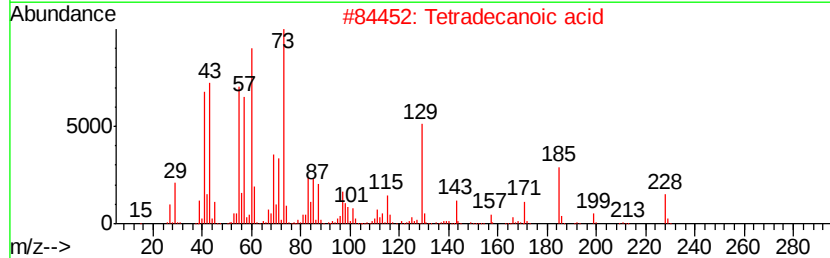
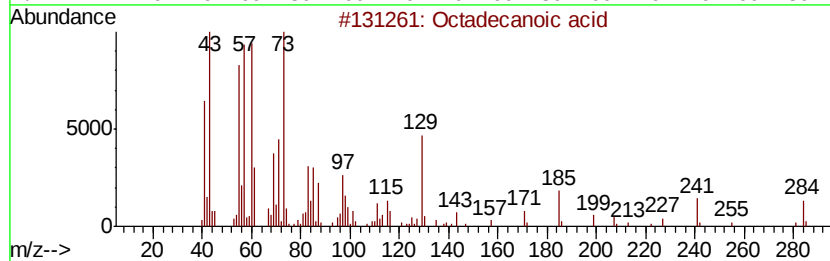
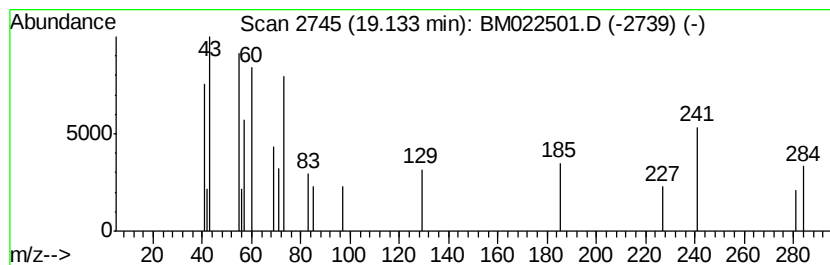
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.13	2.82 ng	29880	Chrysene-d12	21.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	70
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	35
3		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	35
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	35
5		3-Ethylheptanoic acid	158	C9H18O2	014272-47-0	12



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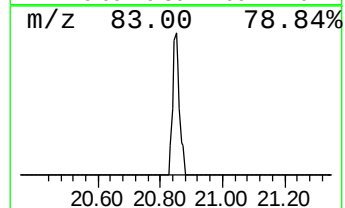
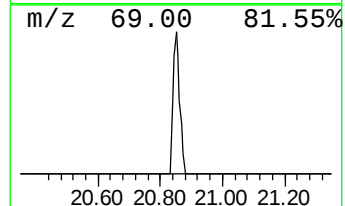
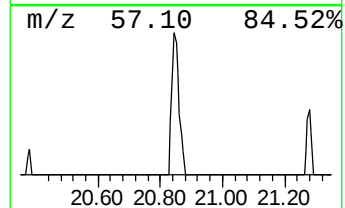
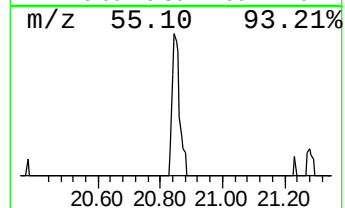
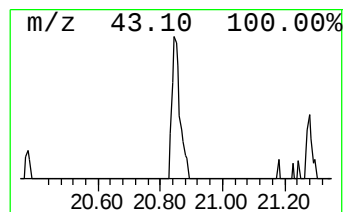
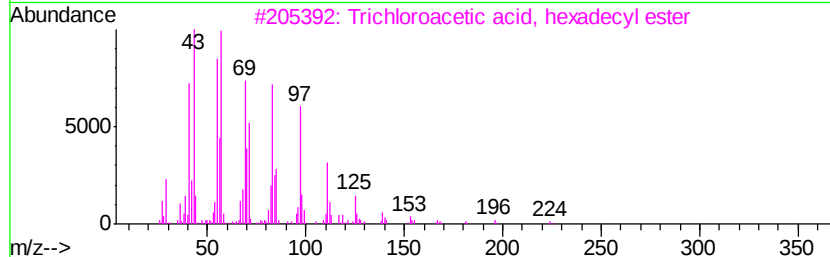
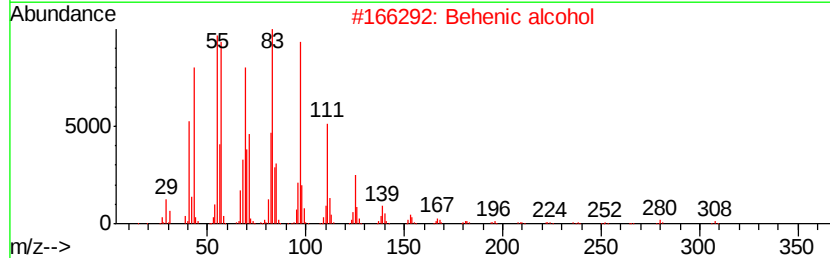
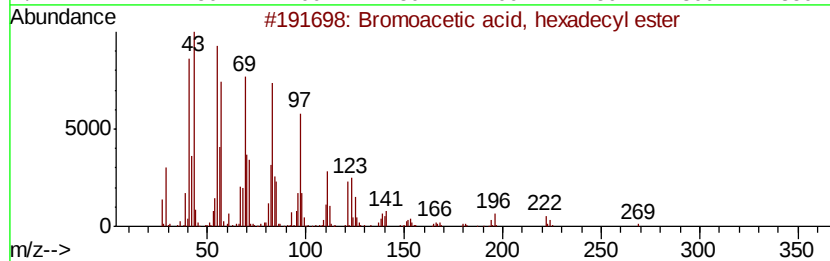
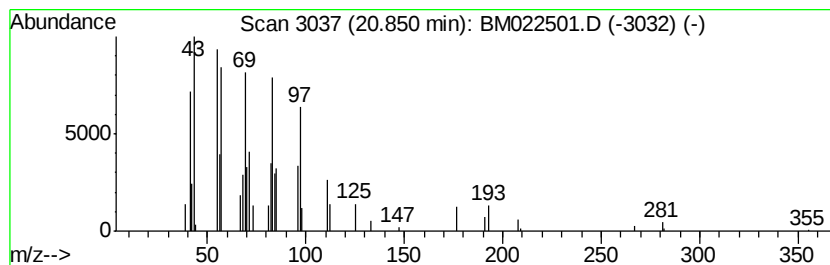
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Peak Number 5 Bromoacetic acid, hexadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.85	4.15 ng	43942	Chrysene-d12	21.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
2		Behenic alcohol	326	C22H46O	000661-19-8	91
3		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
4		Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	90
5		n-Tetracosanol-1	354	C24H50O	000506-51-4	87



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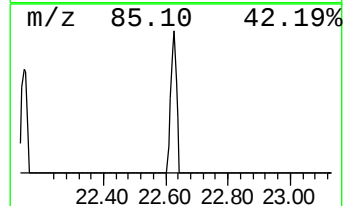
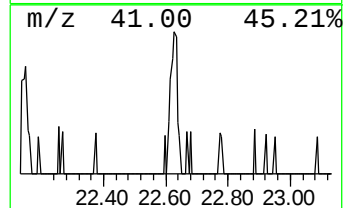
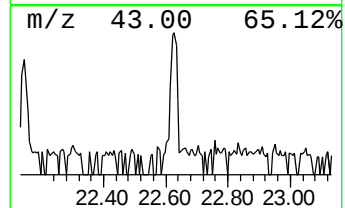
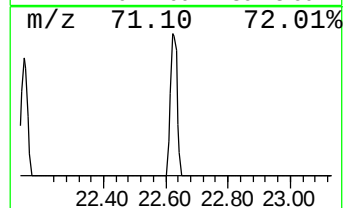
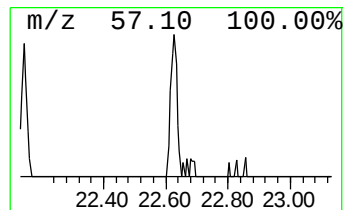
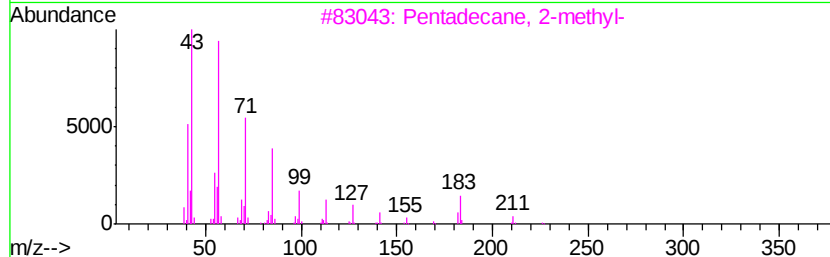
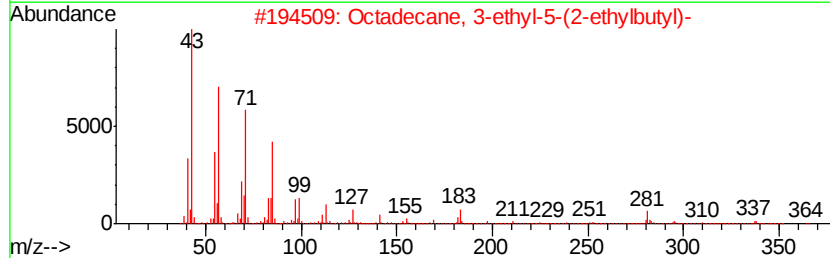
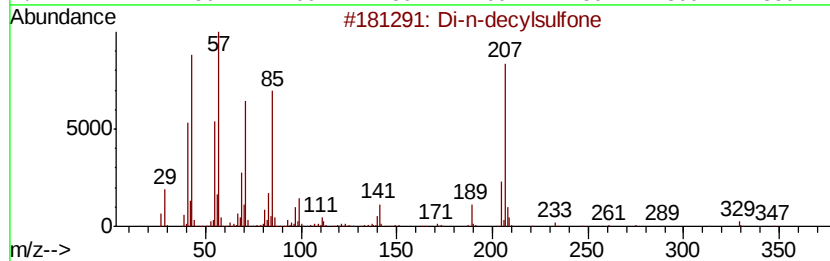
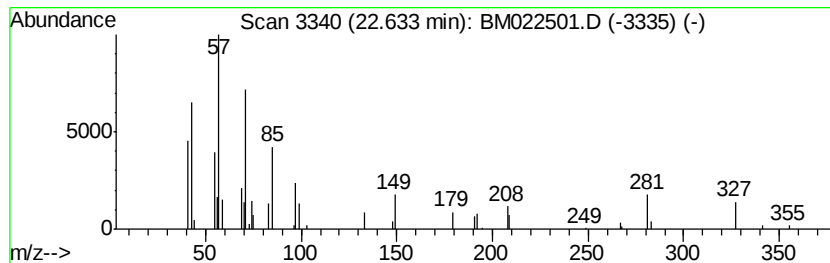
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Peak Number 6 Di-n-decylsulfone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.63	2.43 ng	25743	Perylene-d12	23.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Di-n-decylsulfone	346	C20H42O2S	111530-37-1	53
2		Octadecane, 3-ethyl-5-(2-ethylbu...	366	C26H54	055282-12-7	43
3		Pentadecane, 2-methyl-	226	C16H34	001560-93-6	38
4		Docosane, 11-decyl-	451	C32H66	055401-55-3	38
5		Tricosane, 2-methyl-	338	C24H50	001928-30-9	38



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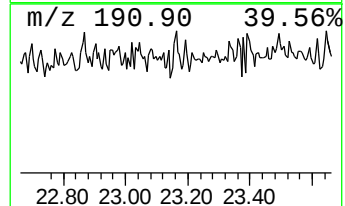
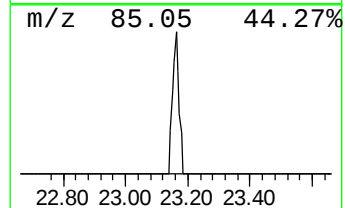
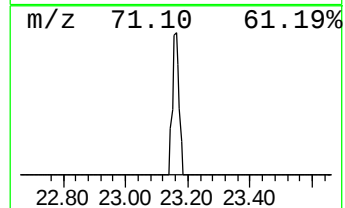
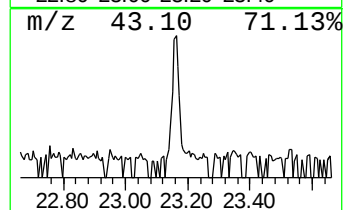
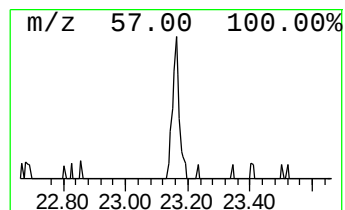
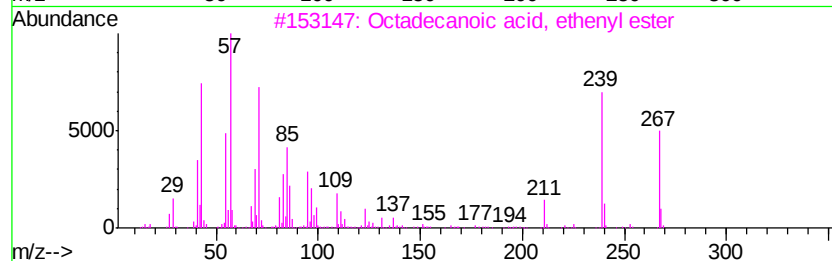
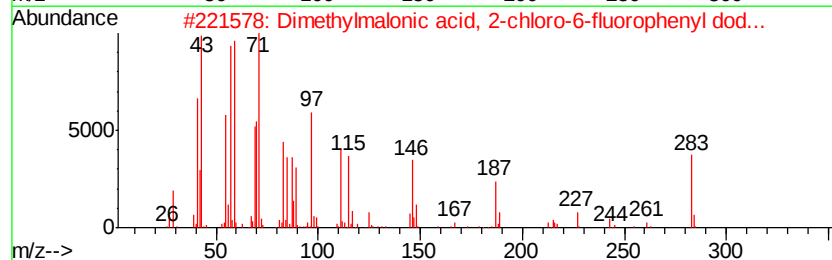
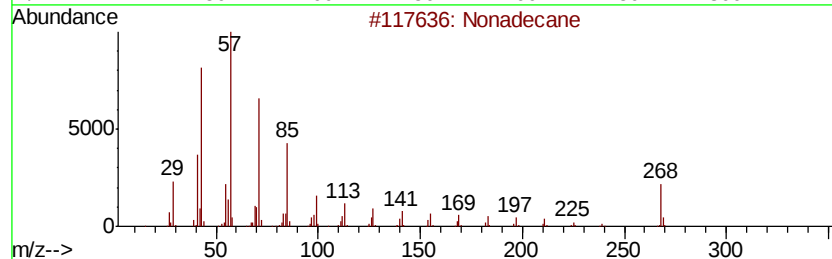
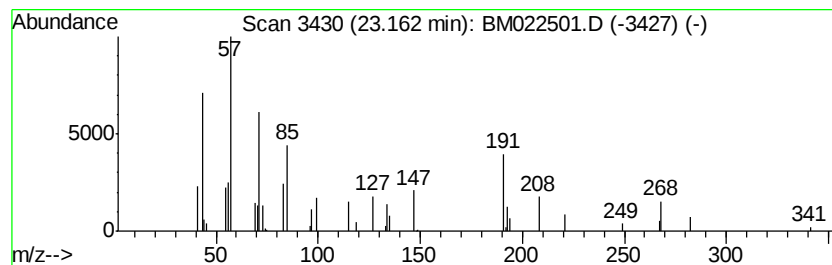
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown23.16 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.16	2.02 ng	21418	Perylene-d12	23.34

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecane	268	C19H40	000629-92-5	38
2		Dimethylmalonic acid, 2-chloro-6...	428	C23H34ClF04	1000361-96-2	9
3		Octadecanoic acid, ethenyl ester	310	C20H38O2	000111-63-7	9
4		Valeric acid, 3,5-dihydroxy-2,4-...	144	C7H12O3	109717-37-5	9
5		Dimethylmalonic acid, dodecyl 2,...	430	C23H33F3O4	1000361-89-0	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA_M\DATA\BM090319\
Data File : BM022501.D
Acq On : 03 Sep 2019 14:04
Operator : HP/JU
Sample : K4619-15
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
TP5-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_M\METHODS\8270-BM082919.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.04	7.04	75.4	ng	446442	1	7.50	118464	20.0
n-Hexadecanoic acid	17.83	7.0	ng	59426	4	16.94	170411	20.0
Octadecanoic acid	19.13	2.8	ng	29880	5	21.16	211876	20.0
Bromoacetic acid,...	20.85	4.2	ng	43942	5	21.16	211876	20.0
Di-n-decylsulfone	22.63	2.4	ng	25743	6	23.34	211726	20.0
unknown23.16	23.16	2.0	ng	21418	6	23.34	211726	20.0