

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
 Data File : BM029324.D
 Acq On : 02 Apr 2021 17:10
 Operator : CG/JU
 Sample : M1874-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_M
 ClientSampleId :
 FS-SB16(7-8)

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-BM040121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029324.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.940	5	9	14	rBV	653263	731645	13.05%	2.339%
2	2.987	14	17	31	rVB	133115	170770	3.04%	0.546%
3	4.846	328	333	342	rVB2	37626	59480	1.06%	0.190%
4	5.298	403	410	420	rBV	2109279	3049070	54.36%	9.746%
5	6.875	670	678	689	rBV	2073774	3244763	57.85%	10.372%
6	7.698	812	818	825	rVB	470045	716468	12.77%	2.290%
7	8.851	1006	1014	1024	rBV	1249329	2041551	36.40%	6.526%
8	10.480	1283	1291	1298	rBV	560961	911079	16.24%	2.912%
9	12.957	1705	1712	1720	rBV	2761452	4029008	71.84%	12.879%
10	13.792	1847	1854	1863	rBV	88436	133251	2.38%	0.426%
11	14.333	1940	1946	1953	rBV	734617	1086802	19.38%	3.474%
12	15.821	2192	2199	2215	rBV	2040785	2912030	51.92%	9.308%
13	17.074	2406	2412	2422	rBV	810640	1202937	21.45%	3.845%
14	17.974	2560	2565	2582	rBV	297263	504924	9.00%	1.614%
15	19.256	2778	2783	2795	rBV	112319	188132	3.35%	0.601%
16	19.698	2852	2858	2864	rBV	4788201	5608609	100.00%	17.928%
17	20.392	2969	2976	2990	rBV	632644	849198	15.14%	2.714%
18	20.968	3070	3074	3083	rBV	537912	726834	12.96%	2.323%
19	21.244	3116	3121	3127	rBV	1162279	1433361	25.56%	4.582%
20	22.291	3296	3299	3304	rVB3	90061	109870	1.96%	0.351%
21	23.456	3491	3497	3504	rVB	874456	1574154	28.07%	5.032%

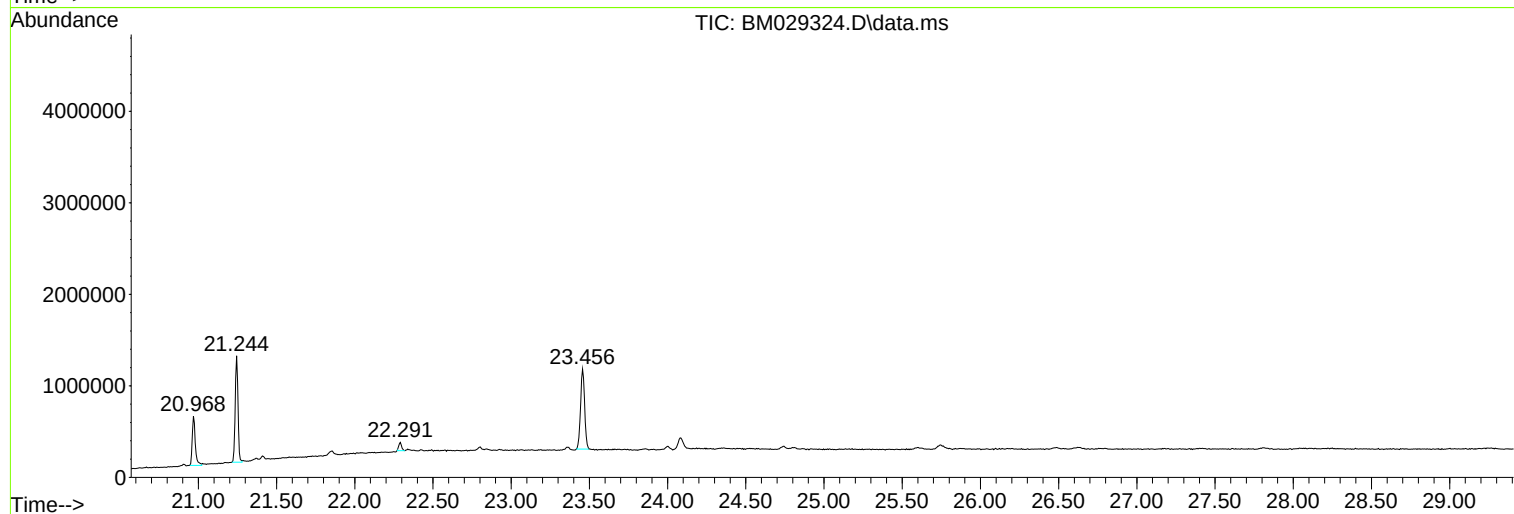
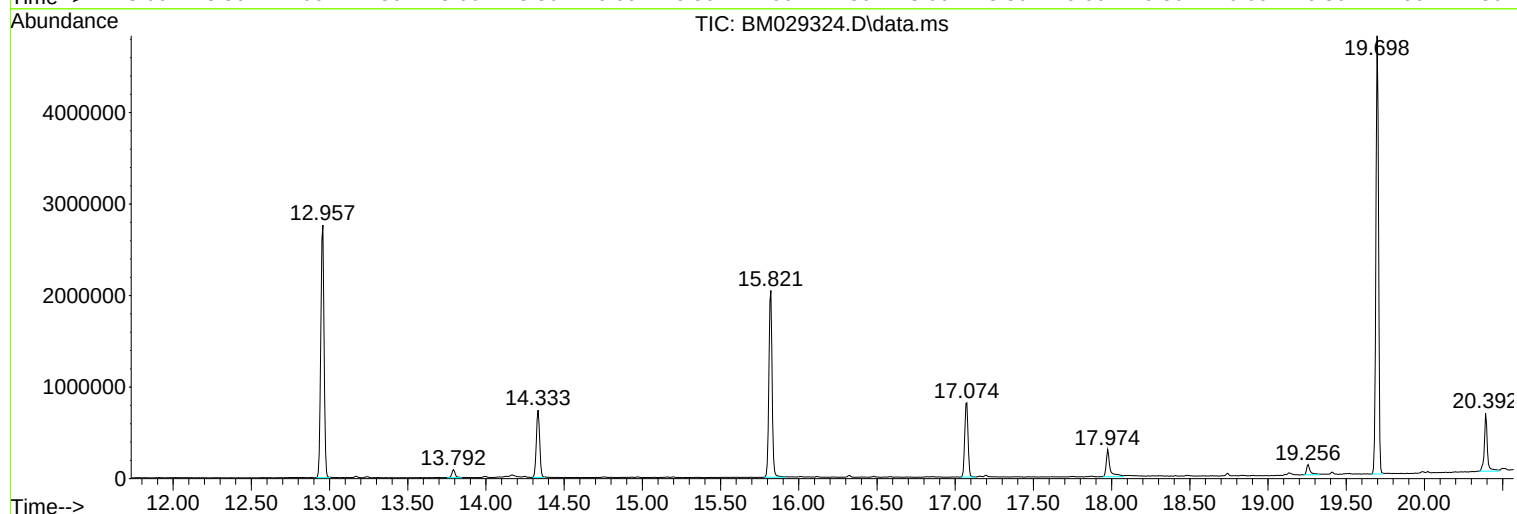
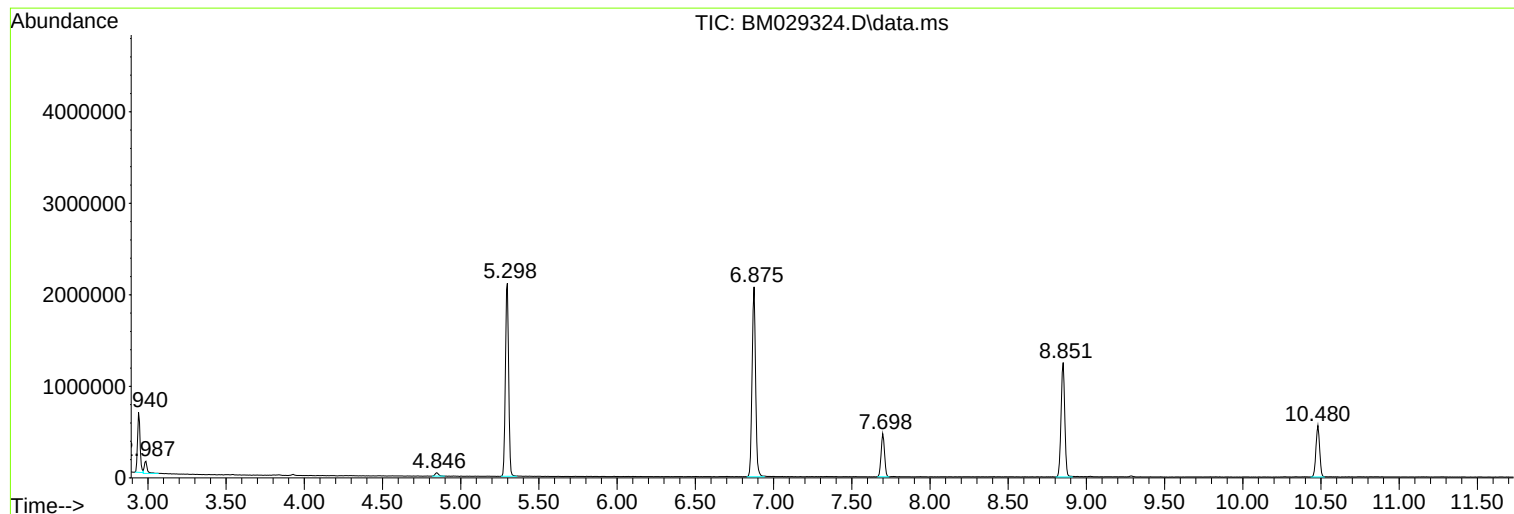
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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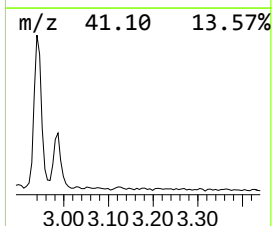
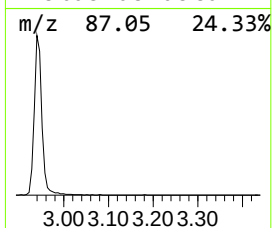
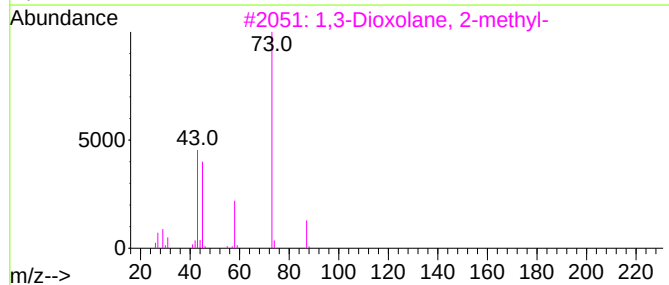
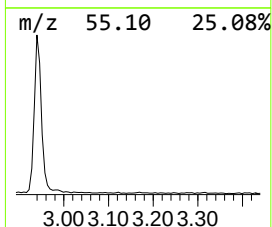
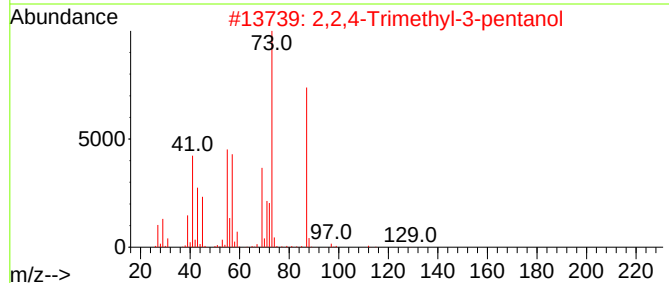
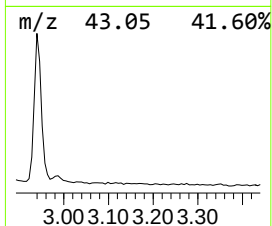
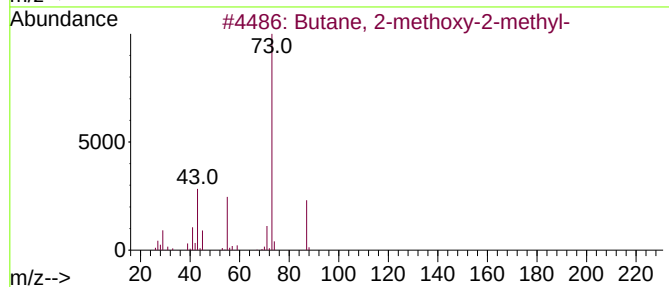
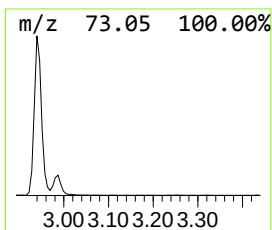
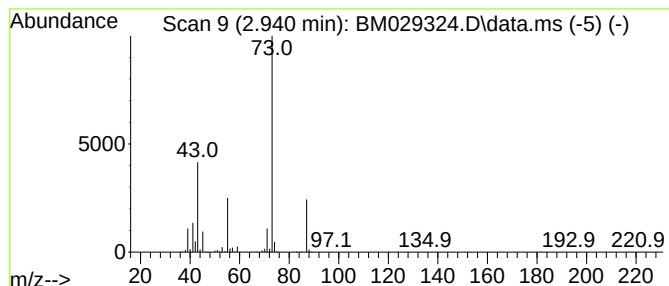
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.940	20.42 ng	731645	1,4-Dichlorobenzene-d4	7.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	10
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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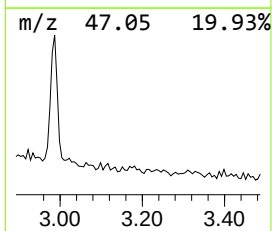
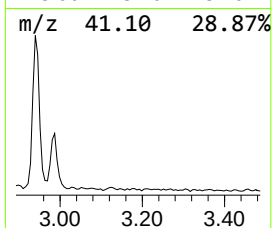
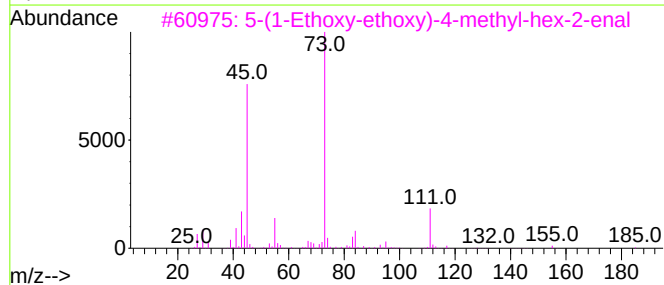
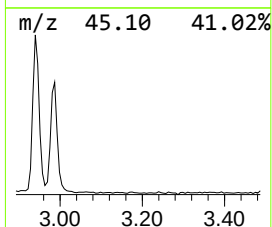
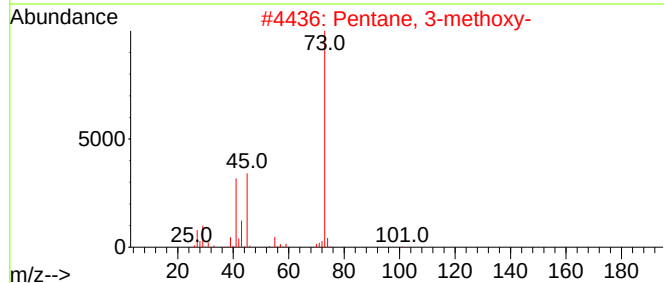
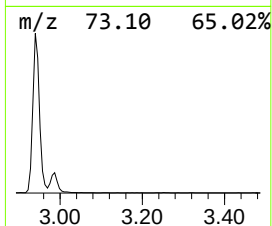
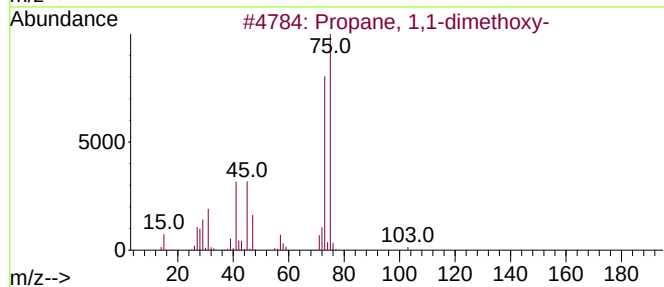
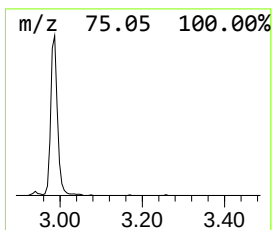
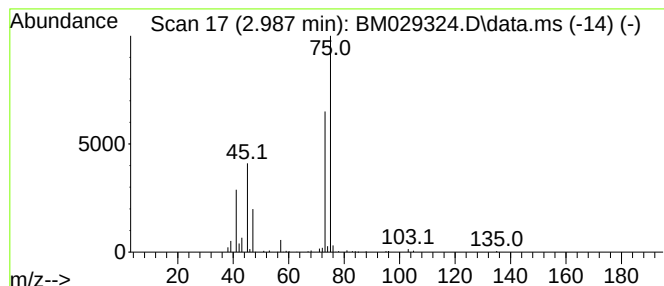
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.98 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.987	4.77 ng	170770	1,4-Dichlorobenzene-d4	7.698

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	38
2			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
3			5-(1-Ethoxy-ethoxy)-4-methyl-hex...	200	C11H20O3	086845-53-6	10
4			Ethanethiol, 2-trimethylsiloxy-	150	C5H14OSSi	037515-85-8	9
5			1-Butanol, 3-(1-ethoxyethoxy)-2-...	176	C9H20O3	059410-44-5	9



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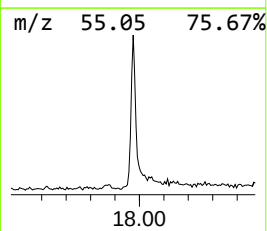
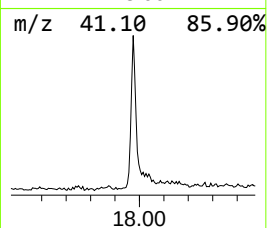
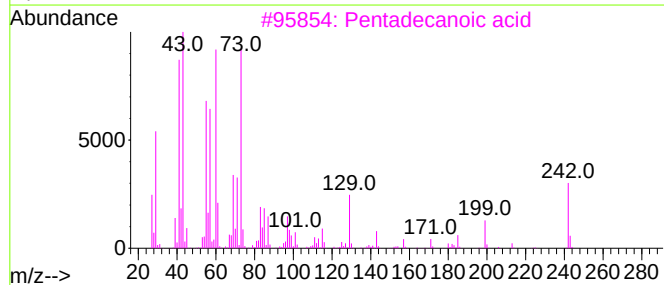
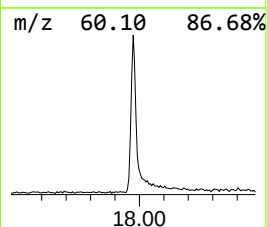
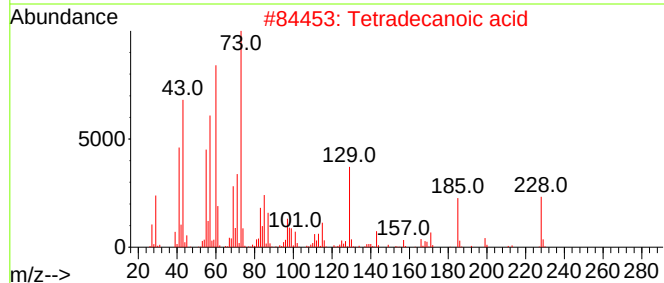
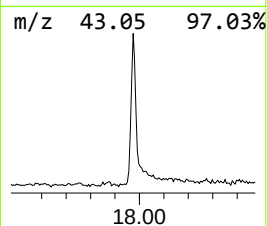
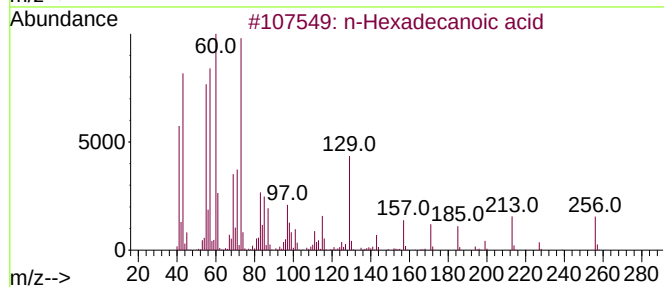
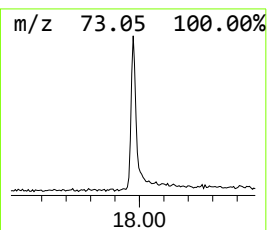
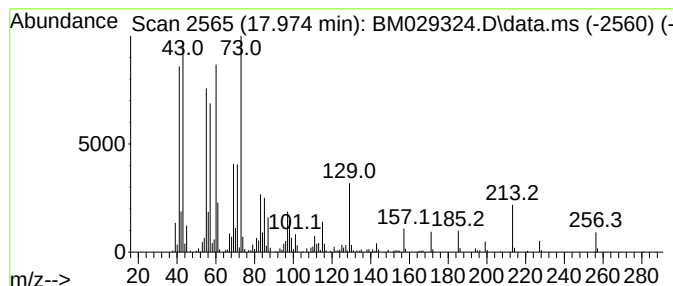
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.974	8.39 ng	504924	Phenanthrene-d10	17.074

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	86
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4			Tridecanoic acid	214	C13H26O2	000638-53-9	70
5			Heptane, 2,6-dimethyl-	128	C9H20	001072-05-5	11



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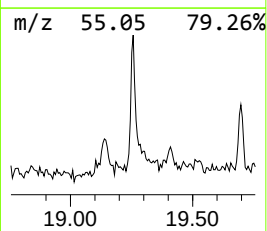
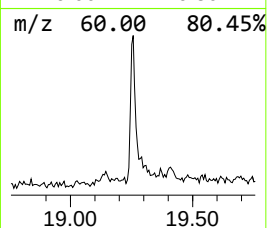
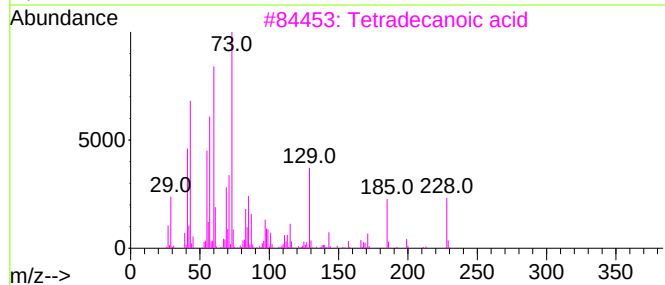
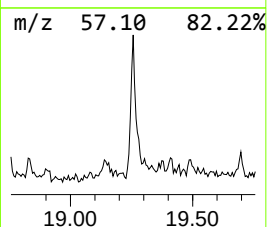
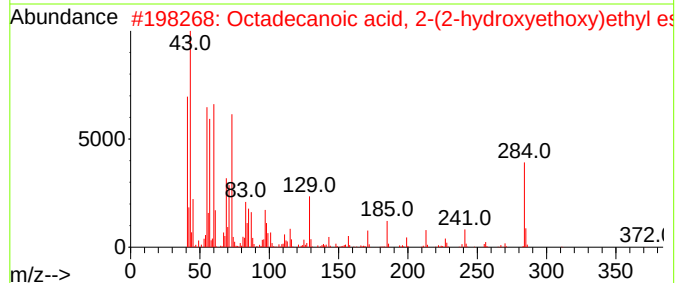
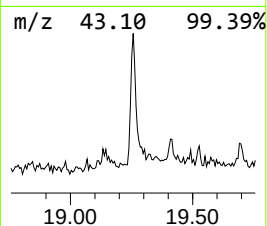
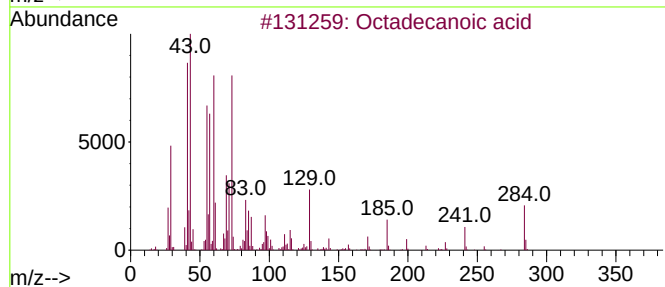
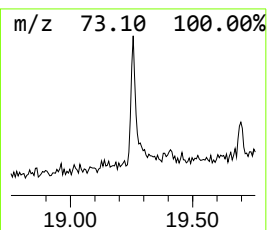
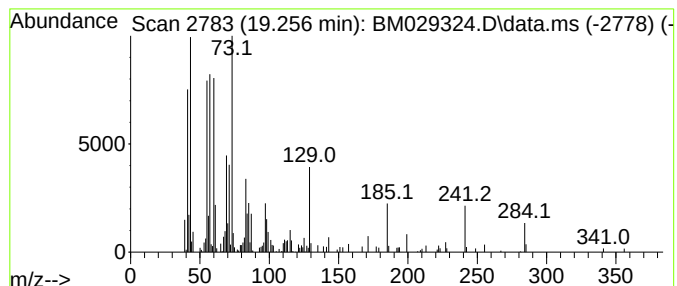
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.256	2.63 ng	188132	Chrysene-d12	21.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	86
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Tridecanoic acid	214	C13H26O2	000638-53-9	59



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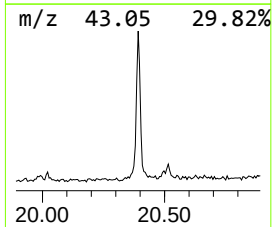
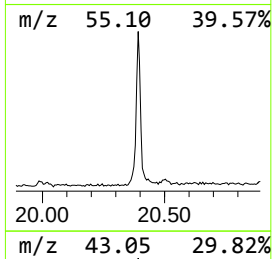
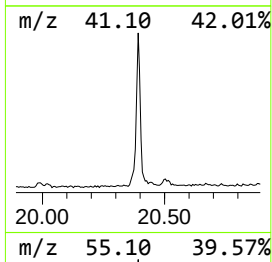
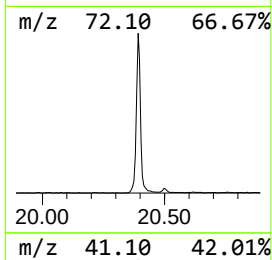
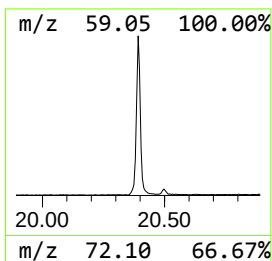
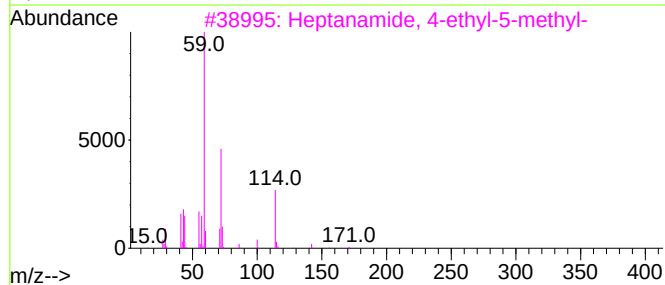
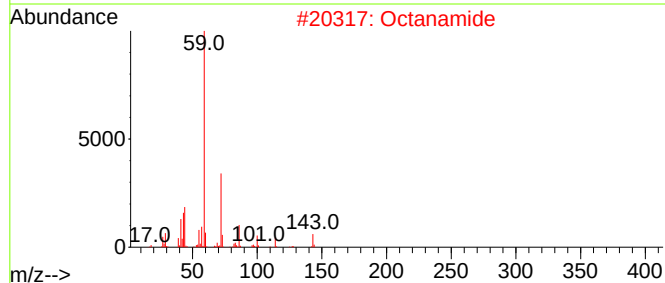
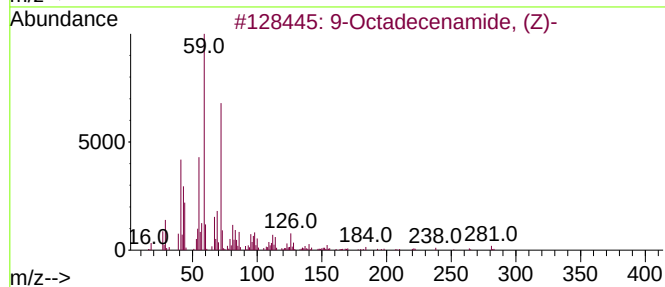
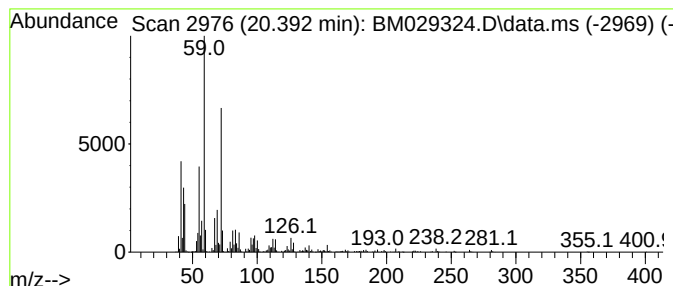
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.392	11.85 ng	849198	Chrysene-d12	21.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2			Octanamide	143	C8H17NO	000629-01-6	72
3			Heptanamide, 4-ethyl-5-methyl-	171	C10H21NO	054789-40-1	64
4			Tetradecanamide	227	C14H29NO	000638-58-4	64
5			Nonanamide	157	C9H19NO	001120-07-6	64



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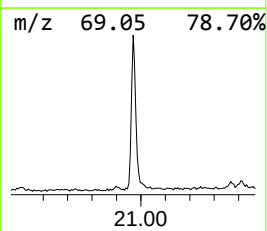
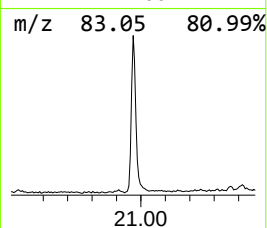
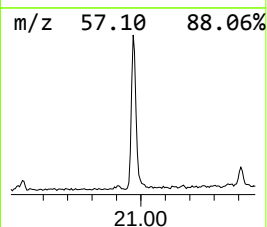
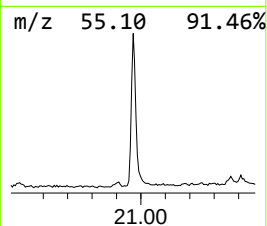
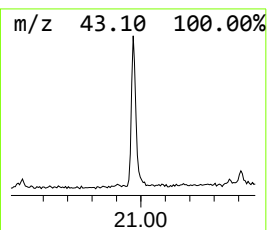
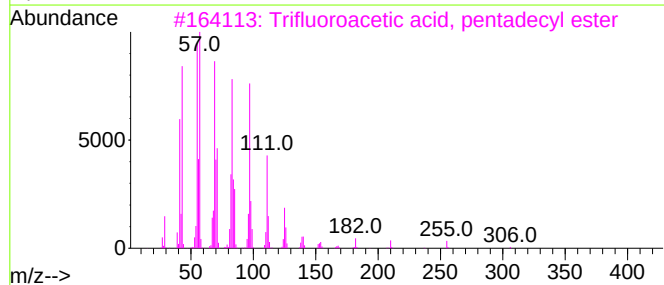
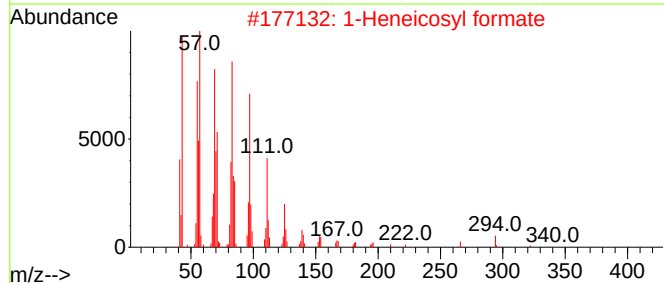
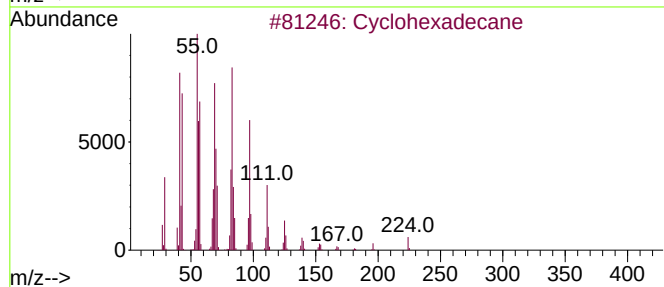
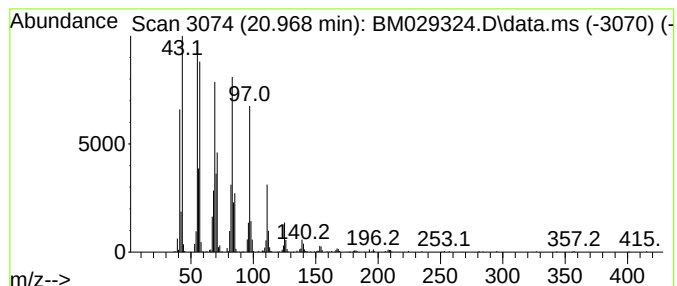
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Cyclohexadecane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.968	10.14 ng	726834	Chrysene-d12	21.244

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexadecane	224	C16H32	000295-65-8	97
2			1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
5			n-Tetracosanol-1	354	C24H50O	000506-51-4	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM040221\
Data File : BM029324.D
Acq On : 02 Apr 2021 17:10
Operator : CG/JU
Sample : M1874-04
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
FS-SB16(7-8)

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM040121.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
Butane, 2-metho...	2.940	20.4	ng	731645	1	7.698	716468	20.0
unknown2.98	2.987	4.8	ng	170770	1	7.698	716468	20.0
n-Hexadecanoic ...	17.974	8.4	ng	504924	4	17.074	1202940	20.0
Octadecanoic acid	19.256	2.6	ng	188132	5	21.244	1433360	20.0
9-Octadecenamid...	20.392	11.9	ng	849198	5	21.244	1433360	20.0
Cyclohexadecane	20.968	10.1	ng	726834	5	21.244	1433360	20.0