

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042825\
 Data File : BP024446.D
 Acq On : 28 Apr 2025 21:06
 Operator : RC/JU
 Sample : Q1895-05
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 COMP-3

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_P\Methods\8270E-BP041425.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP024446.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.875	299	304	313	rBV	187896	265895	2.53%	0.615%
2	5.334	375	382	397	rBV	2239148	3142216	29.92%	7.262%
3	6.905	639	649	665	rBV	2111605	3371061	32.10%	7.791%
4	7.716	777	787	796	rBV	438889	726721	6.92%	1.680%
5	8.863	974	982	994	rBV	1260298	2111538	20.11%	4.880%
6	10.481	1249	1257	1269	rBV	586930	1013968	9.66%	2.343%
7	12.951	1670	1677	1694	rBV	4368720	5475207	52.14%	12.654%
8	14.345	1905	1914	1929	rBV	1029675	1466727	13.97%	3.390%
9	15.734	2144	2150	2155	rBV	541212	683079	6.50%	1.579%
10	15.857	2165	2171	2190	rBV2	4247240	5850179	55.71%	13.520%
11	17.145	2383	2390	2402	rBV2	1143629	1878432	17.89%	4.341%
12	18.086	2544	2550	2563	rBV2	364407	665613	6.34%	1.538%
13	18.528	2621	2625	2632	rVB	97527	128883	1.23%	0.298%
14	19.339	2756	2763	2772	rBV	299763	618295	5.89%	1.429%
15	19.416	2772	2776	2789	rVB	167150	308036	2.93%	0.712%
16	19.875	2848	2854	2862	rVB	8024652	10501468	100.00%	24.270%
17	21.257	3085	3089	3102	rVB2	174222	377178	3.59%	0.872%
18	21.586	3139	3145	3152	rBV2	1478077	2396825	22.82%	5.539%
19	24.921	3705	3712	3729	rVB	884937	2288287	21.79%	5.288%

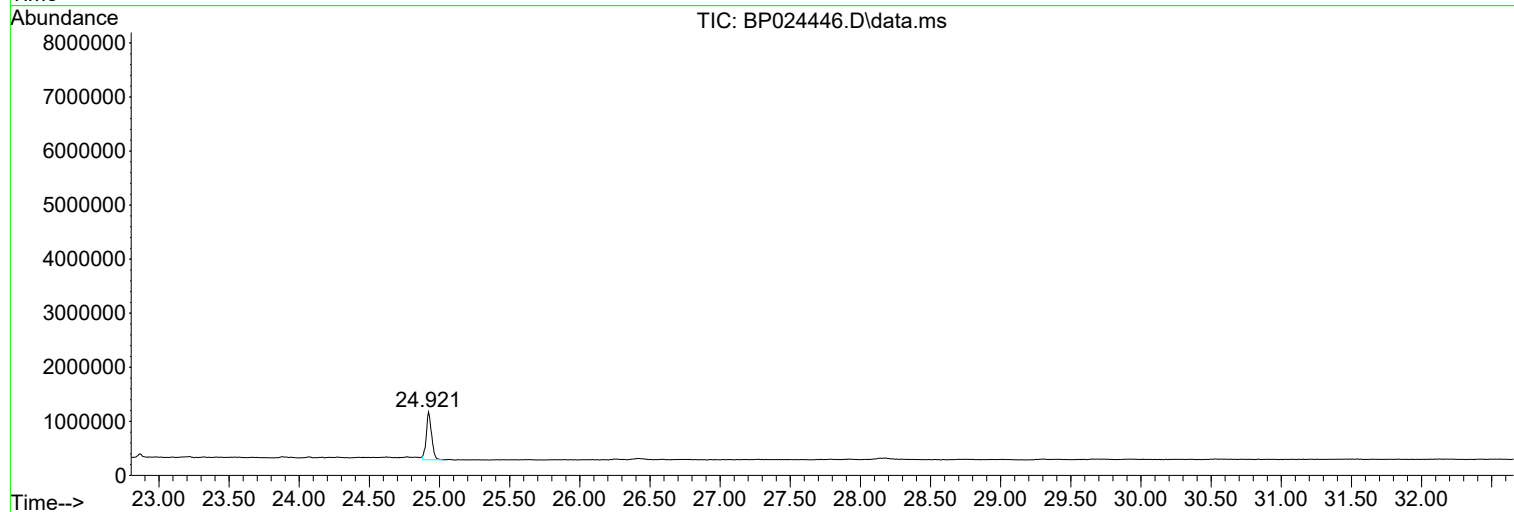
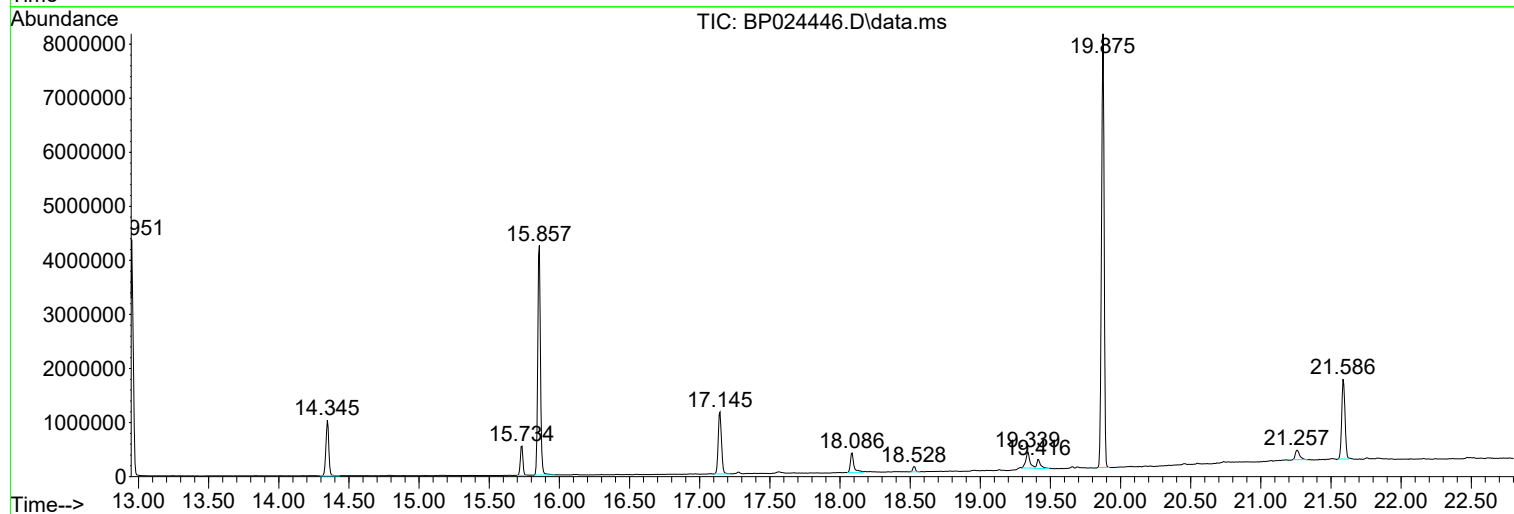
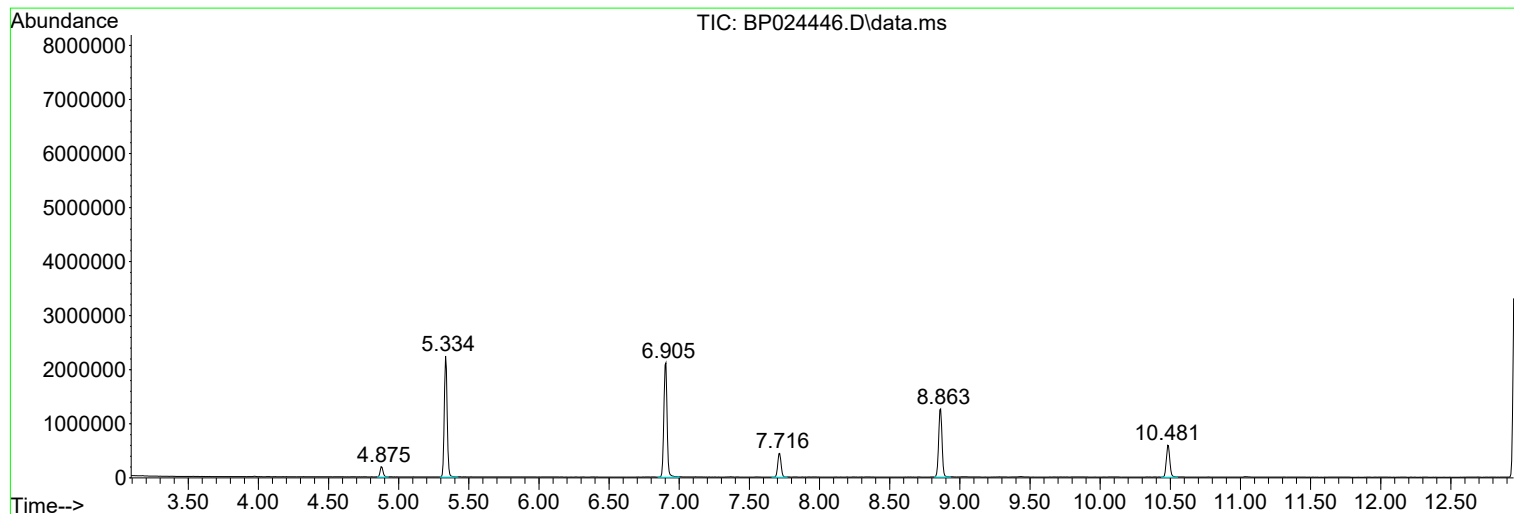
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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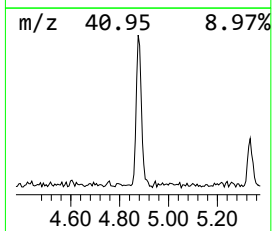
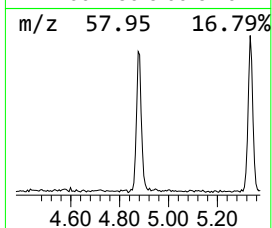
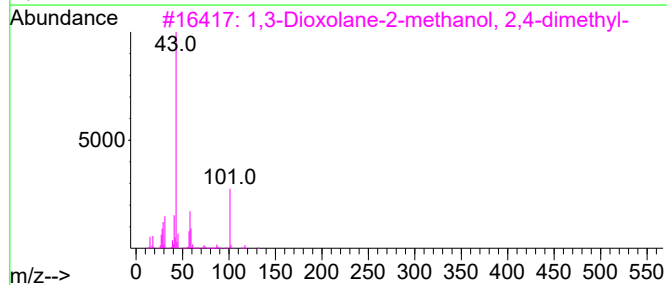
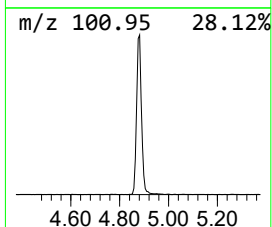
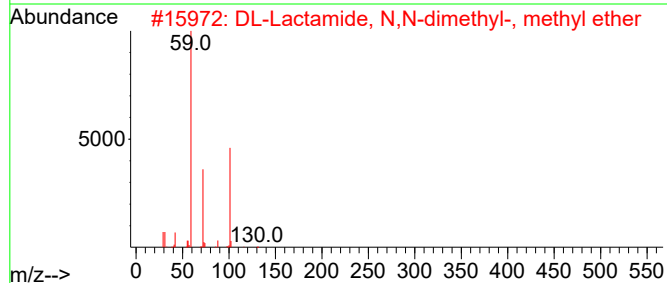
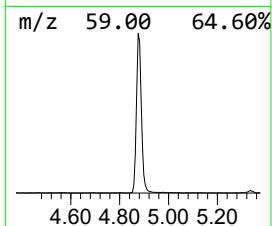
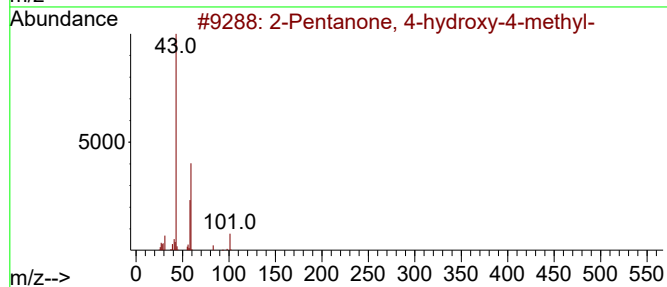
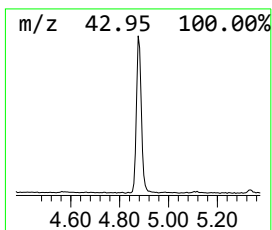
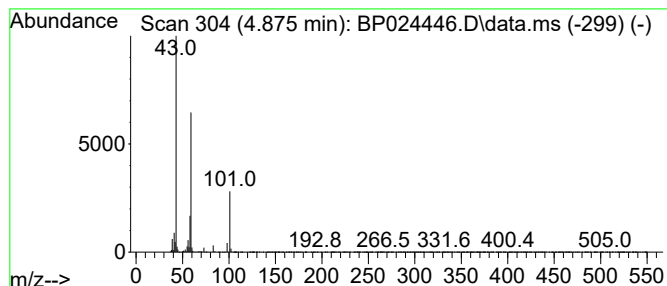
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.875	7.32 ng	265895	1,4-Dichlorobenzene-d4	7.716

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	DL-Lactamide, N,N-dimethyl-, met...	131	C6H13NO2	1000452-57-0	33		
3	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25		
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25		
5	4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23		



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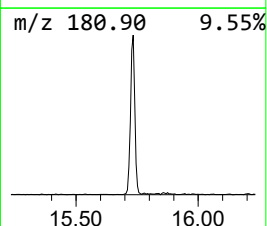
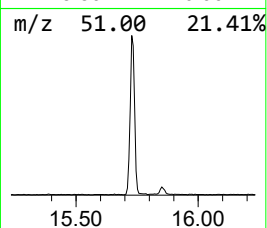
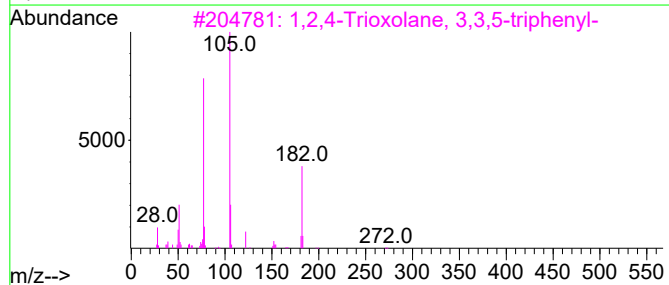
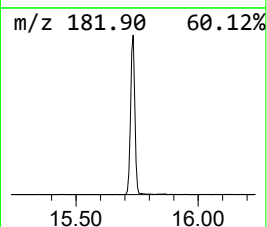
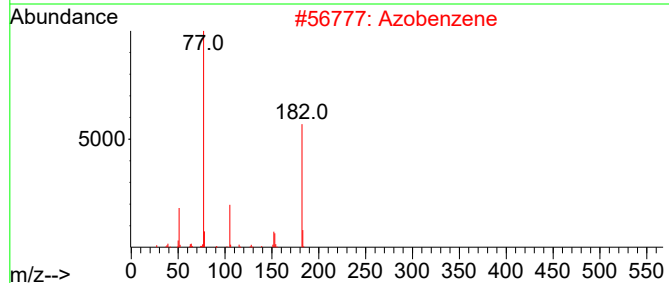
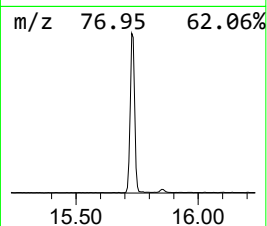
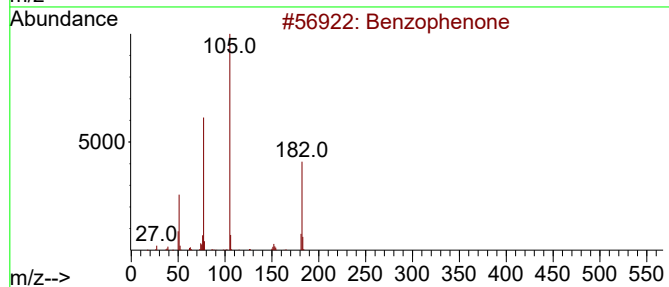
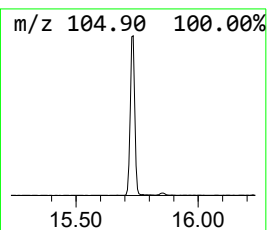
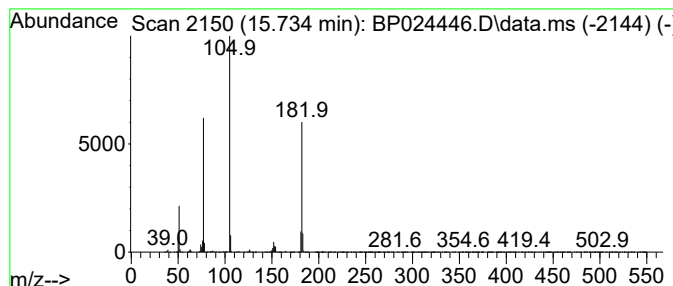
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Peak Number 2 Benzophenone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.734	9.31 ng	683079	Acenaphthene-d10	14.345

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	97
2			Azobenzene	182	C12H10N2	000103-33-3	53
3			1,2,4-Trioxolane, 3,3,5-triphenyl-	304	C20H16O3	023246-12-0	50
4			Benzenamine, N-(3-pyridinylmethy...	182	C12H10N2	029722-97-2	42
5			1,2,4-Triazolo[4,3-b]pyridazine,...	182	C7H7ClN4	028593-26-2	38



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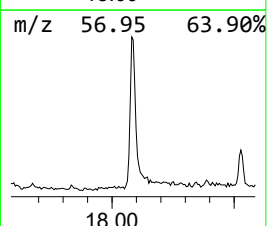
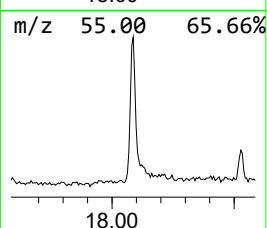
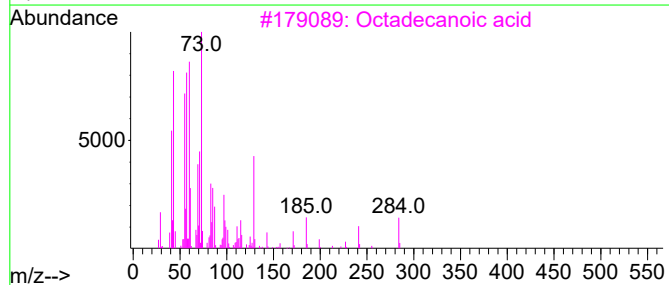
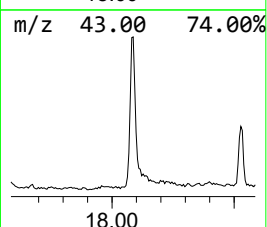
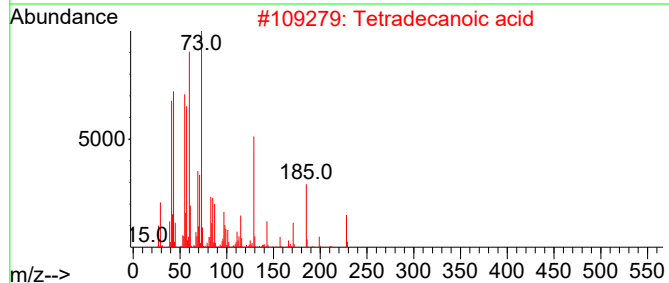
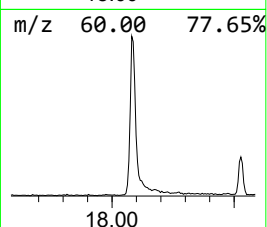
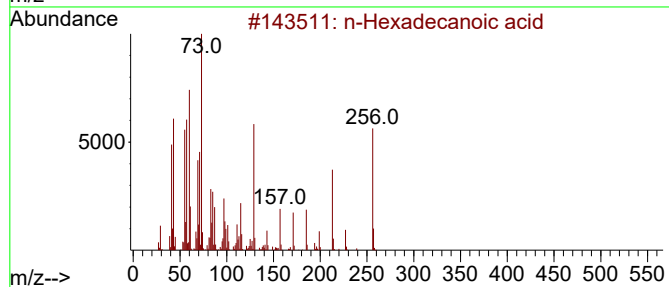
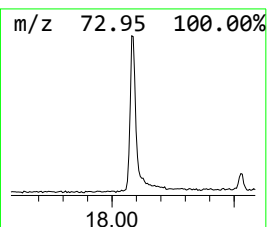
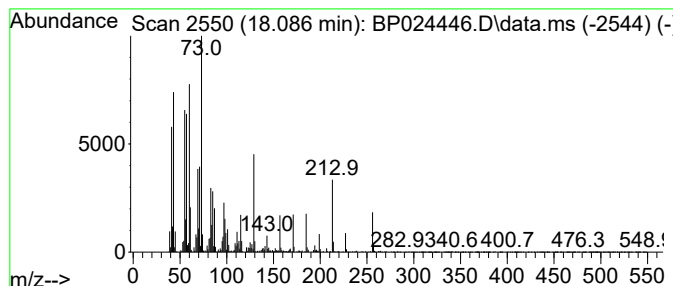
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Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.086	7.09 ng	665613	Phenanthrene-d10	17.145

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	91
3			Octadecanoic acid	284	C18H36O2	000057-11-4	90
4			Tridecanoic acid	214	C13H26O2	000638-53-9	89
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	87



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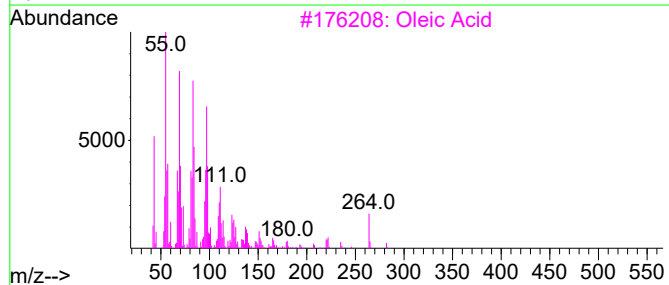
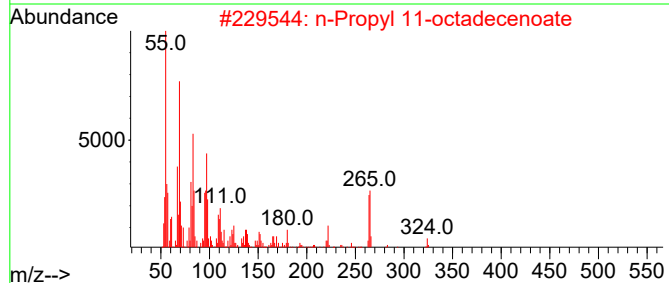
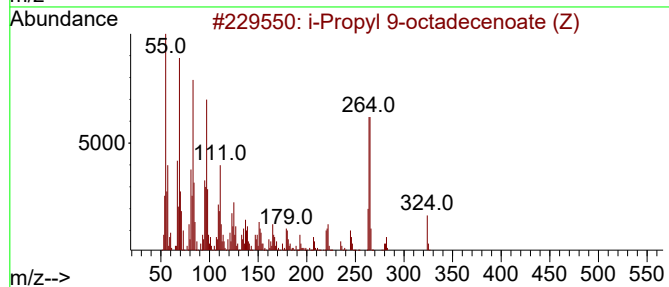
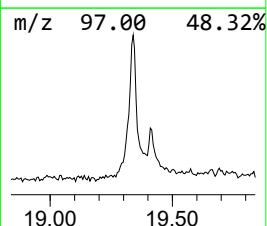
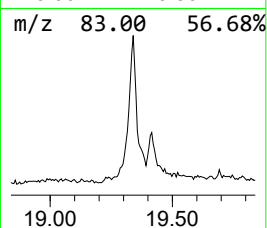
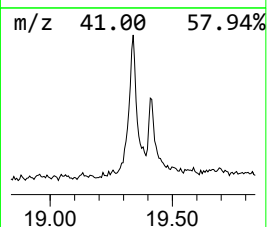
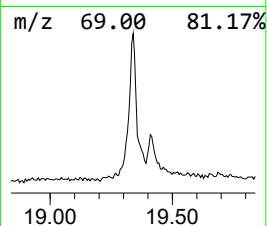
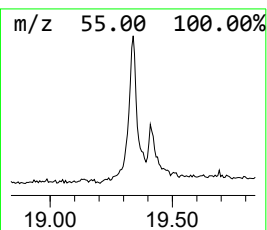
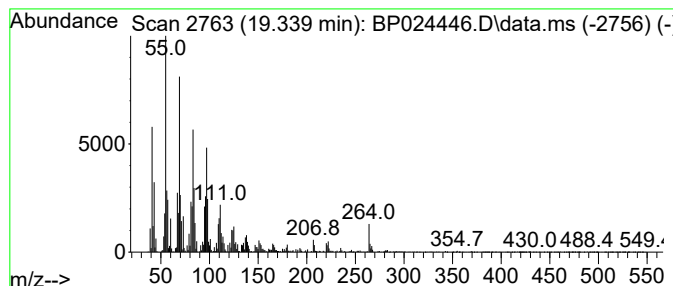
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 i-Propyl 9-octadecenoate (Z) Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	6.58 ng	618295	Phenanthrene-d10	17.145

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			i-Propyl 9-octadecenoate (Z)	324	C21H40O2	000112-11-8	91
2			n-Propyl 11-octadecenoate	324	C21H40O2	1000336-71-7	91
3			Oleic Acid	282	C18H34O2	000112-80-1	87
4			9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	87
5			cis-Vaccenic acid	282	C18H34O2	000506-17-2	86



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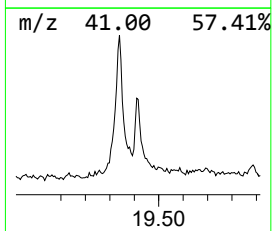
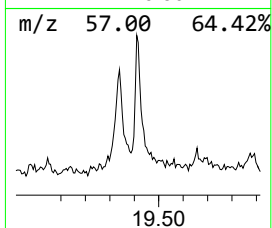
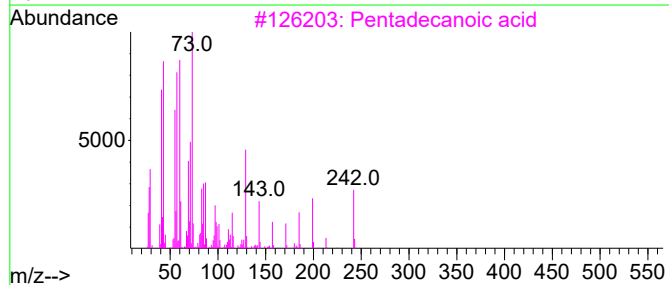
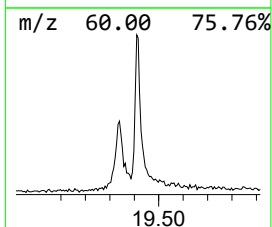
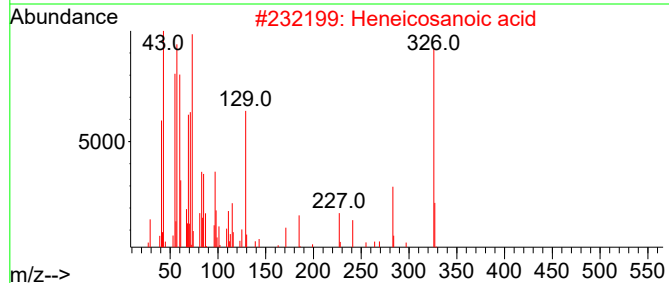
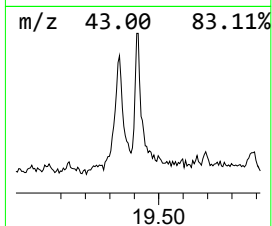
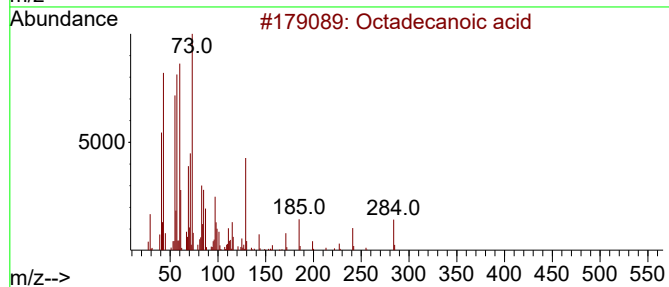
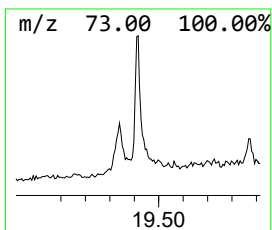
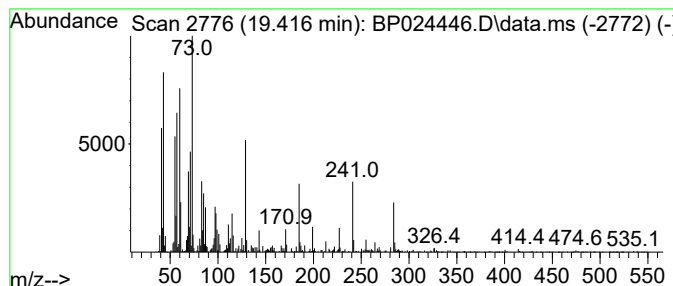
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.416	2.57 ng	308036	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Heneicosanoic acid	326	C21H42O2	002363-71-5	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4			n-Decanoic acid	172	C10H20O2	000334-48-5	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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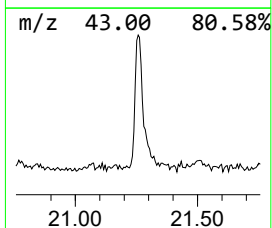
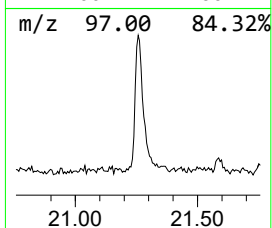
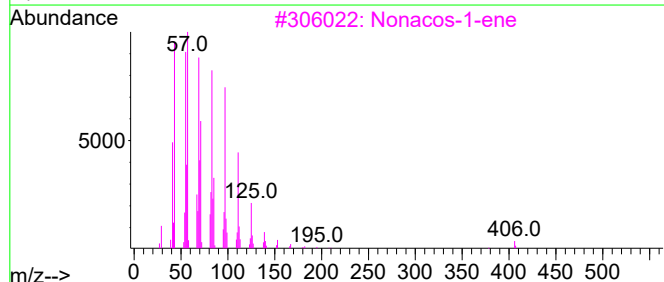
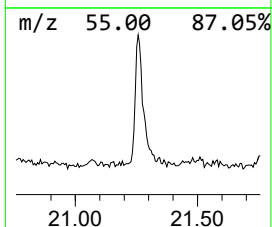
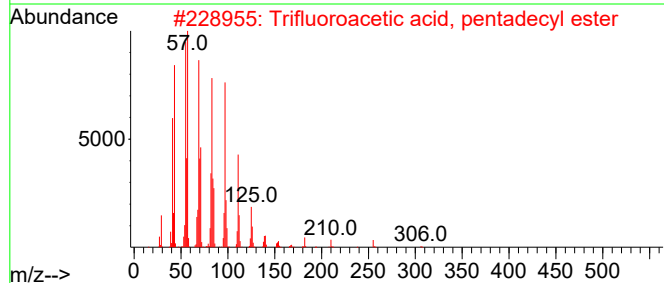
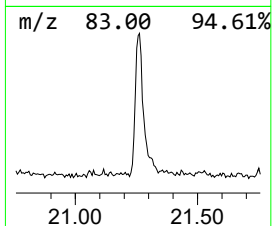
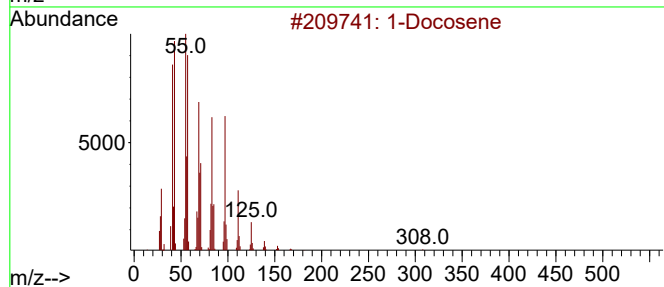
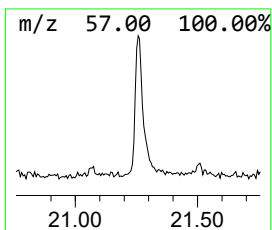
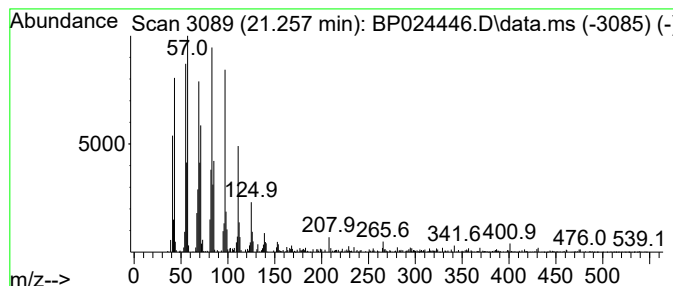
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.257	3.15 ng	377178	Chrysene-d12	21.586

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Docosene	308	C22H44	001599-67-3	94
2			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3			Nonacos-1-ene	406	C29H58	018835-35-3	94
4			Pentacos-1-ene	350	C25H50	016980-85-1	94
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP042825\
Data File : BP024446.D
Acq On : 28 Apr 2025 21:06
Operator : RC/JU
Sample : Q1895-05
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
COMP-3

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP041425.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	4.875	7.3	ng	265895	1	7.716	726721	20.0
Benzophenone	15.734	9.3	ng	683079	3	14.345	1466730	20.0
n-Hexadecanoic ...	18.086	7.1	ng	665613	4	17.145	1878430	20.0
i-Propyl 9-octa...	19.339	6.6	ng	618295	4	17.145	1878430	20.0
Octadecanoic acid	19.416	2.6	ng	308036	5	21.586	2396830	20.0
1-Docosene	21.257	3.1	ng	377178	5	21.586	2396830	20.0