

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022324\
 Data File : BP019849.D
 Acq On : 23 Feb 2024 18:21
 Operator : MA/JU
 Sample : P1537-13
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 13

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-BP013124.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP019849.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	323	329	342	rBV	263453	405443	9.58%	1.638%
2	5.481	400	407	417	rBV	1137436	1718934	40.61%	6.946%
3	7.081	669	679	694	rBV	1066688	1792583	42.35%	7.244%
4	7.905	809	819	826	rBV	299977	487471	11.52%	1.970%
5	9.075	1010	1018	1031	rBV	828432	1456200	34.40%	5.884%
6	9.552	1088	1099	1106	rBV	154844	313724	7.41%	1.268%
7	10.704	1285	1295	1304	rBV	406172	724865	17.12%	2.929%
8	12.522	1594	1604	1615	rBV2	24278	76676	1.81%	0.310%
9	13.169	1707	1714	1731	rBV	1826127	2758466	65.17%	11.147%
10	13.445	1753	1761	1771	rBV	986424	1611683	38.08%	6.513%
11	14.545	1940	1948	1961	rBV	531230	840412	19.85%	3.396%
12	14.769	1976	1986	1992	rBV2	72178	168588	3.98%	0.681%
13	16.045	2195	2203	2220	rBV	1642586	2528450	59.73%	10.217%
14	17.310	2410	2418	2422	rBV	682409	1021709	24.14%	4.129%
15	17.351	2422	2425	2431	rVB	68624	99817	2.36%	0.403%
16	18.022	2535	2539	2545	rVB	119174	161329	3.81%	0.652%
17	18.204	2566	2570	2579	rBV	473040	660449	15.60%	2.669%
18	18.369	2594	2598	2608	rVB5	19277	52924	1.25%	0.214%
19	19.322	2756	2760	2769	rVB	243185	370925	8.76%	1.499%
20	19.445	2777	2781	2790	rVB2	168268	243335	5.75%	0.983%
21	19.675	2817	2820	2829	rVB	189041	272615	6.44%	1.102%
22	19.880	2850	2855	2868	rVB	3432692	4232814	100.00%	17.104%
23	21.133	3065	3068	3075	rBV2	267880	330802	7.82%	1.337%
24	21.416	3111	3116	3120	rBV	904785	1276759	30.16%	5.159%
25	23.851	3524	3530	3537	rVB	547835	1140101	26.93%	4.607%

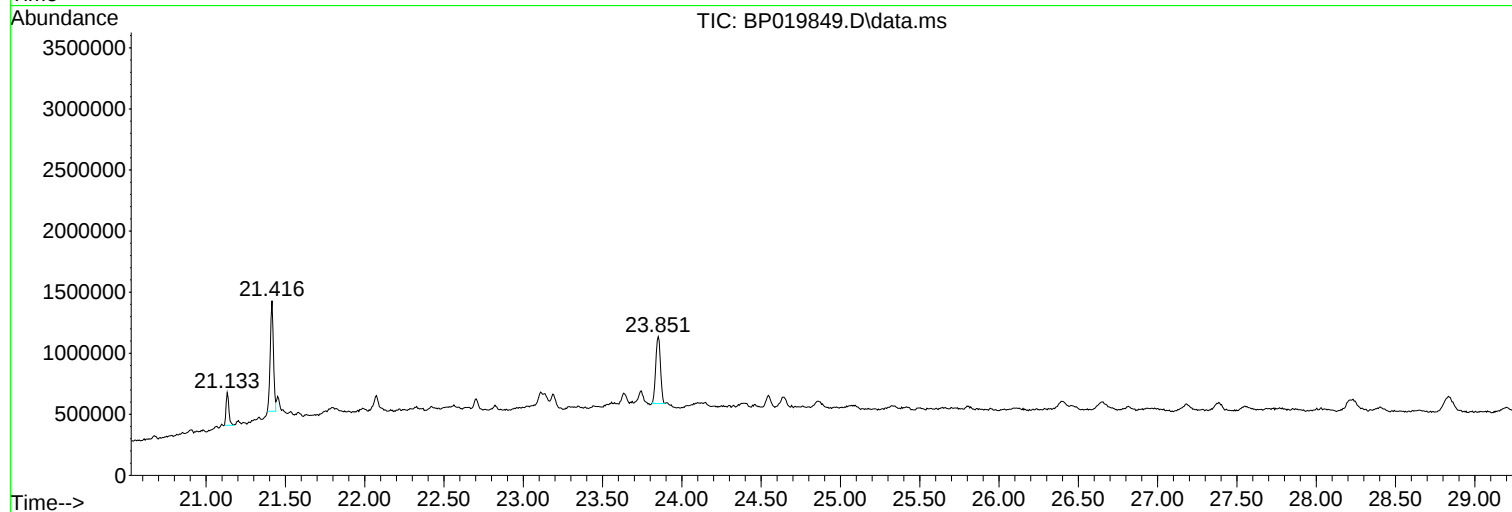
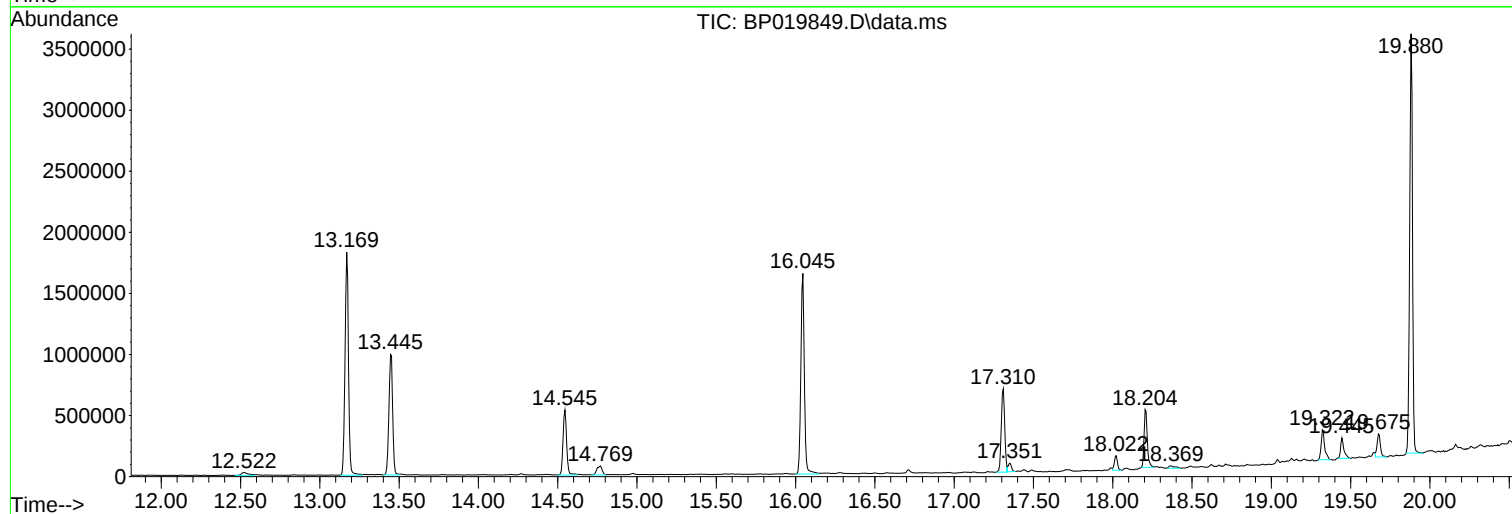
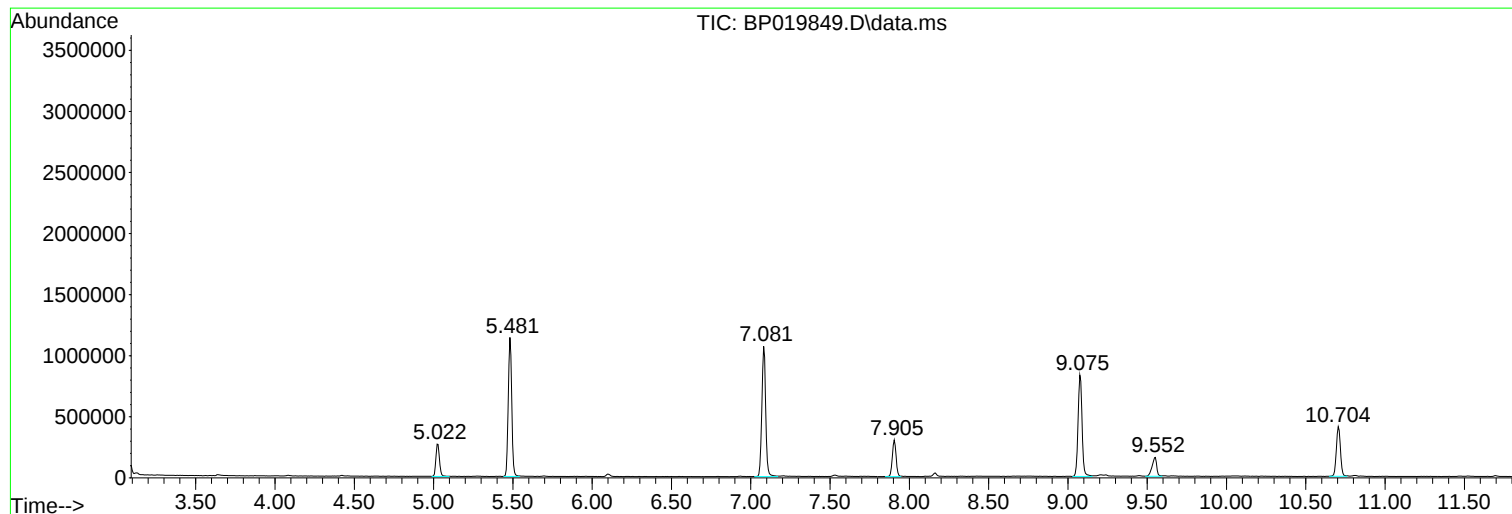
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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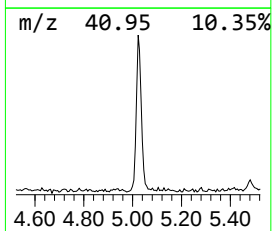
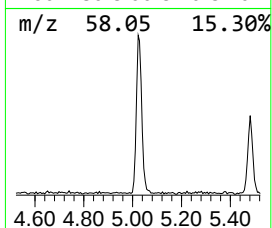
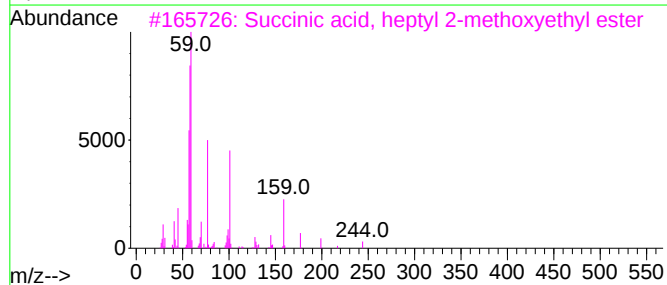
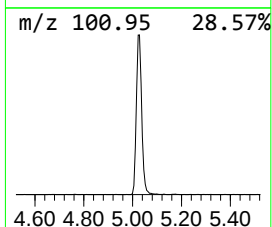
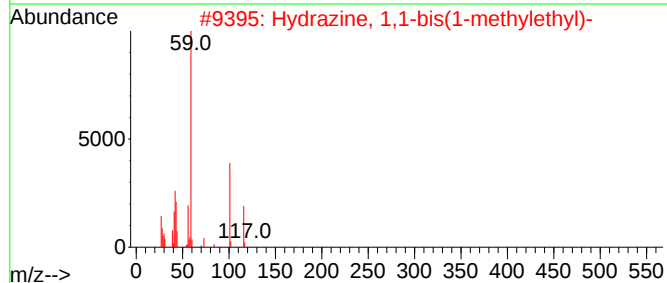
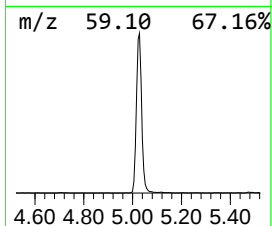
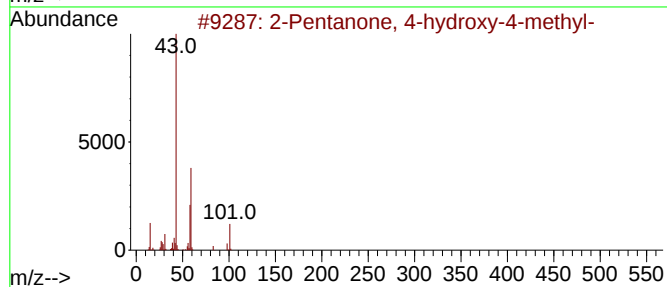
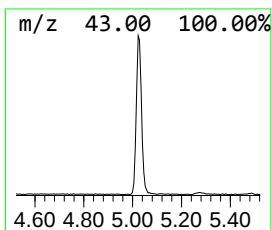
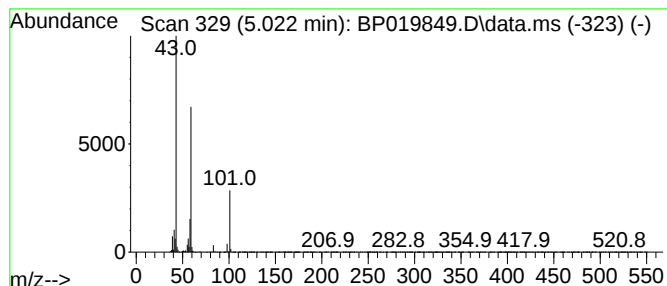
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.022	16.63 ng	405443	1,4-Dichlorobenzene-d4	7.905

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72		
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	47		
3	Succinic acid, heptyl 2-methoxye...	274	C14H26O5	1000325-80-7	28		
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25		
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23		



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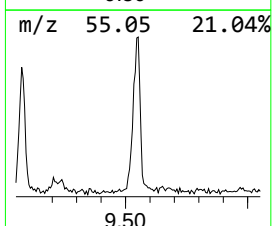
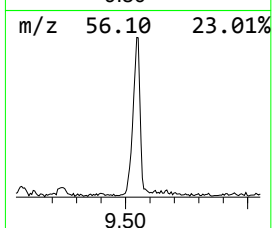
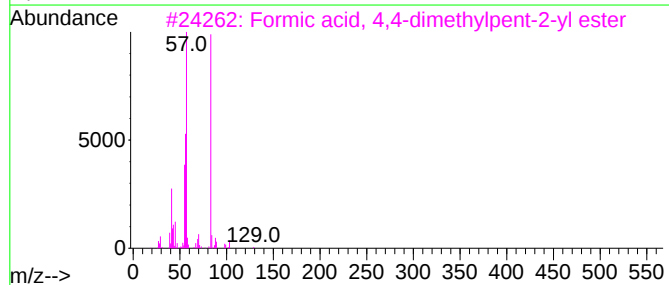
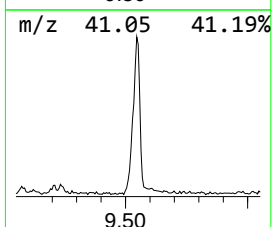
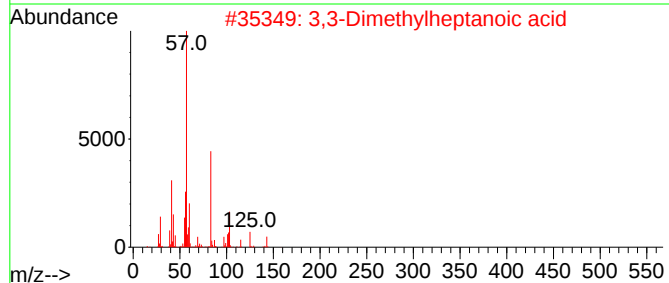
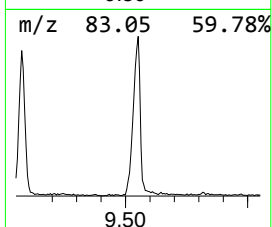
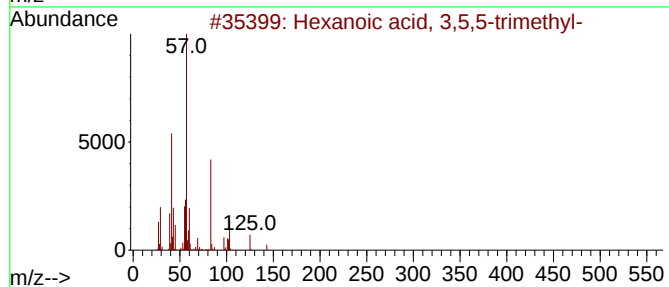
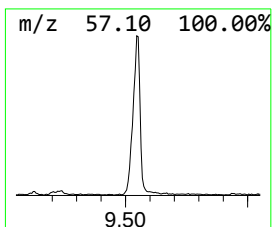
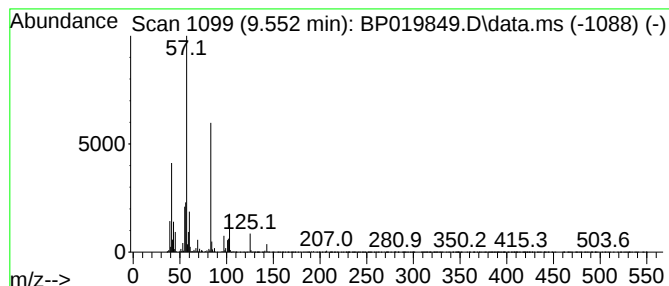
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexanoic acid, 3,5,5-trimet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.552	8.66 ng	313724	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3			Formic acid, 4,4-dimethylpent-2-...	144	C8H16O2	1000368-69-9	37
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	32
5			6,6-Dimethylheptanoic acid	158	C9H18O2	015898-92-7	32



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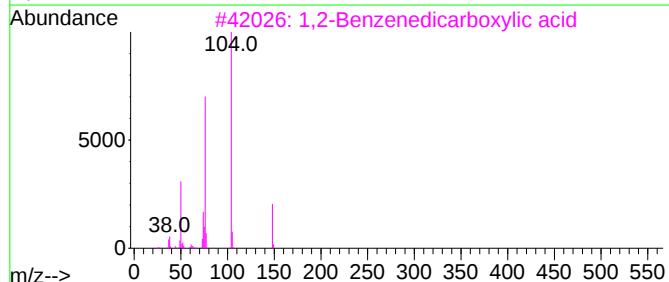
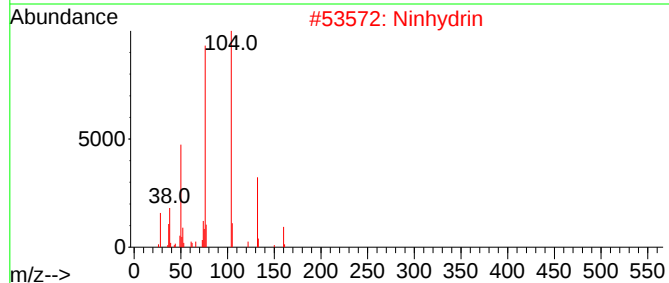
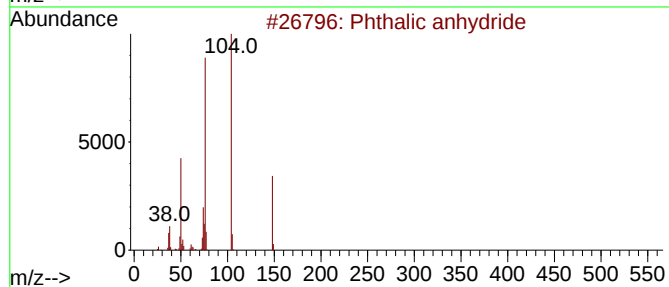
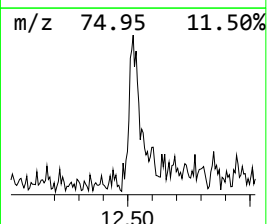
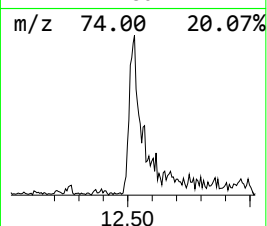
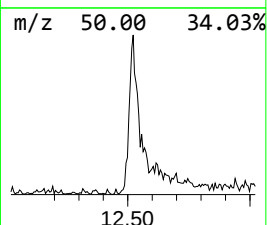
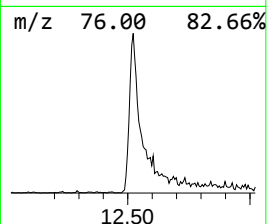
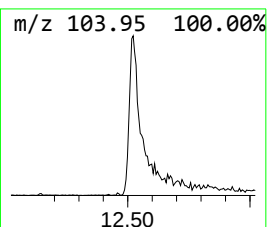
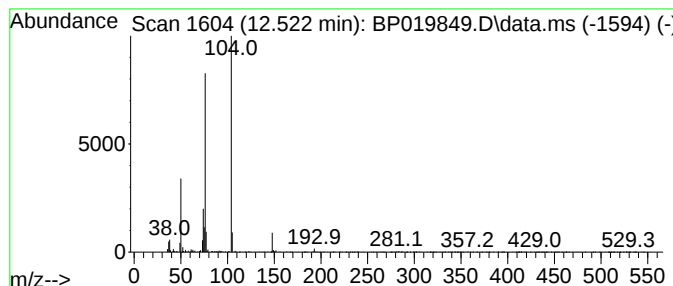
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 Phthalic anhydride Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.522	2.12 ng	76676	Naphthalene-d8	10.704

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phthalic anhydride	148	C8H4O3	000085-44-9	94
2			Ninhydrin	178	C9H6O4	000485-47-2	83
3			1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	83
4			Bicyclo[4.2.0]octa-1,3,5-triene...	132	C8H4O2	006383-11-5	78
5			1H-Isoindole-1,3(2H)-dione, 2-(h...	177	C9H7NO3	000118-29-6	78



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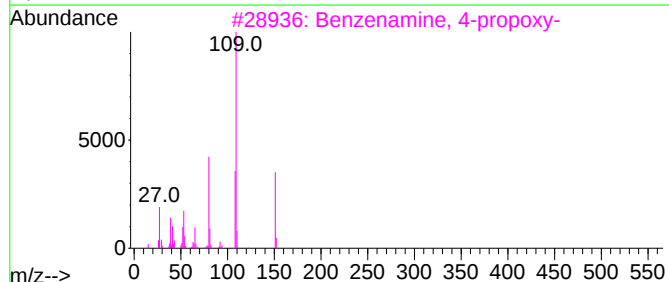
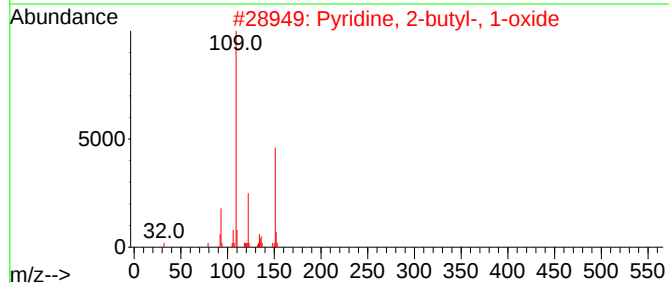
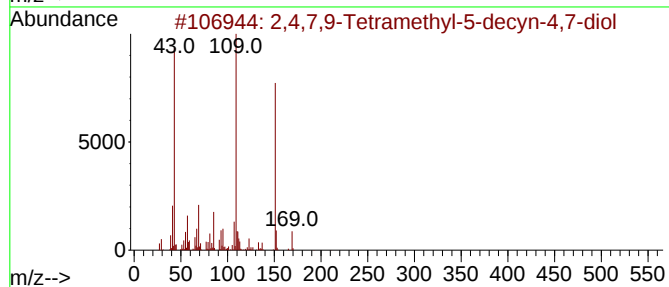
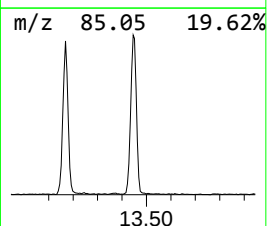
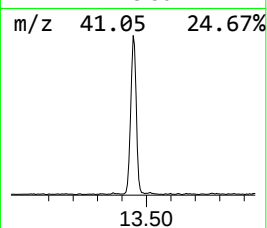
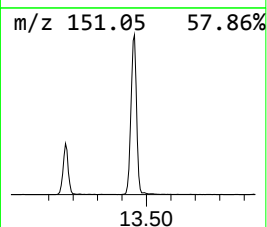
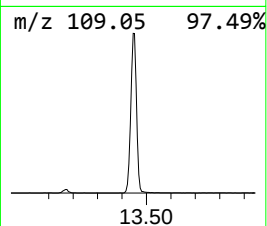
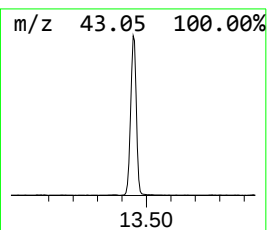
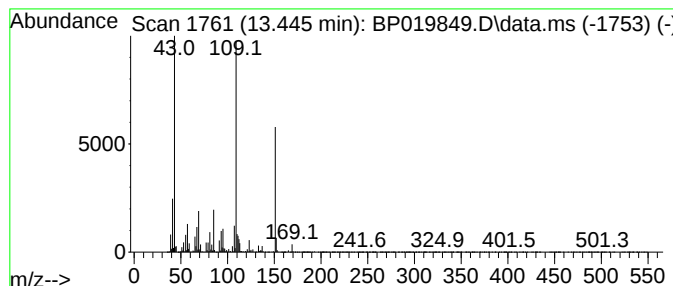
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Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.445	38.35 ng	1611680	Acenaphthene-d10	14.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2	000126-86-3	90		
2	Pyridine, 2-butyl-, 1-oxide	151	C9H13NO	031396-32-4	50		
3	Benzenamine, 4-propoxy-	151	C9H13NO	004469-80-1	50		
4	Acetaminophen	151	C8H9NO2	000103-90-2	50		
5	Metacetamol	151	C8H9NO2	000621-42-1	50		



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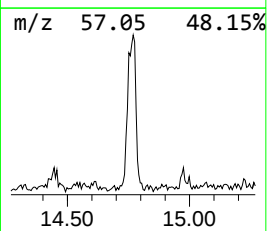
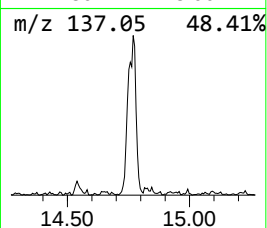
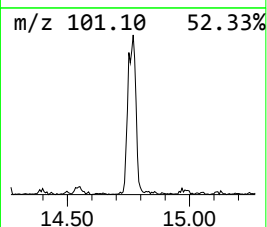
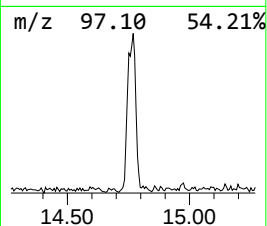
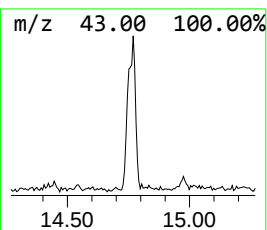
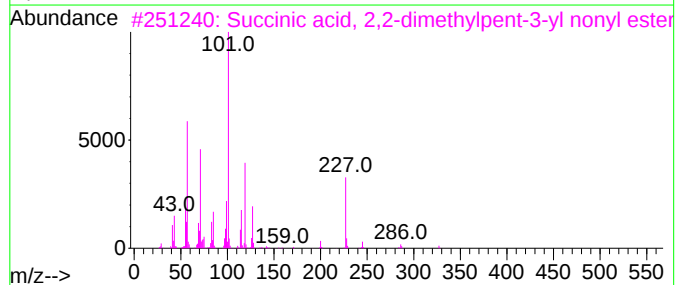
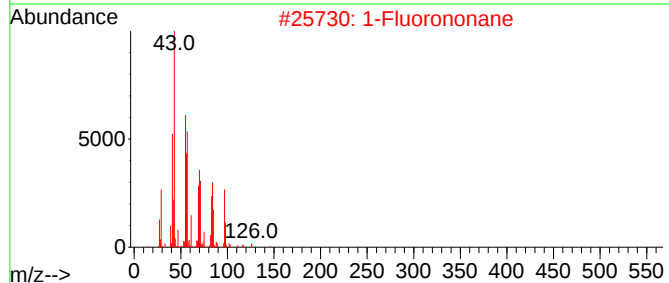
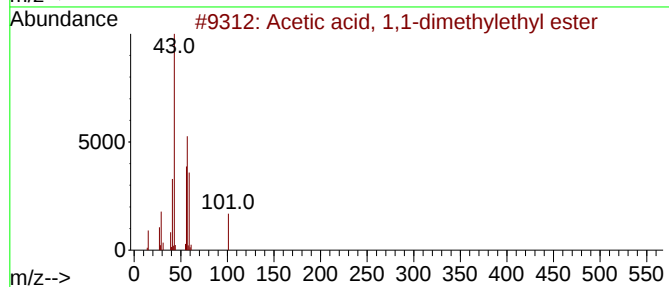
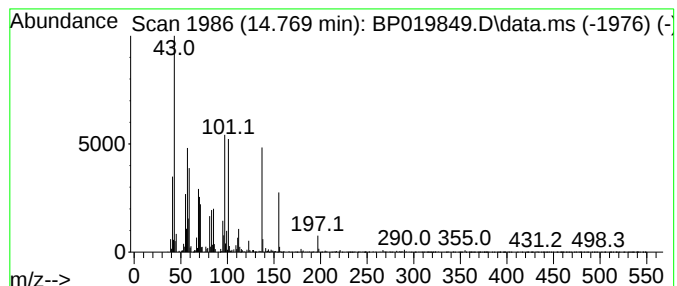
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Peak Number 5 unknown14.769 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.769	4.01 ng	168588	Acenaphthene-d10	14.545

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
2			1-Fluorononane	146	C9H19F	000463-18-3	14
3			Succinic acid, 2,2-dimethylpent-...	342	C20H38O4	1000381-73-7	10
4			Succinic acid, 2-ethylhexyl 4-he...	328	C19H36O4	1000390-47-4	10
5			Succinic acid, cyclohexyl propyl...	242	C13H22O4	1000330-01-3	10



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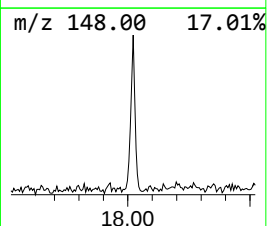
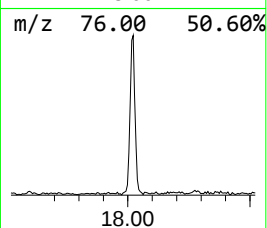
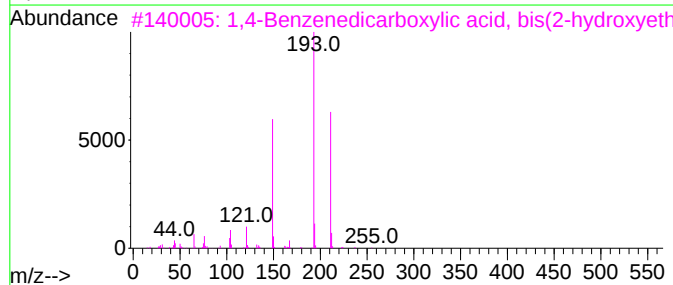
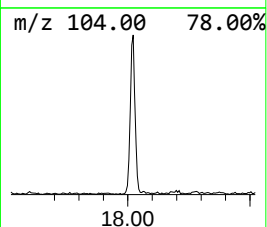
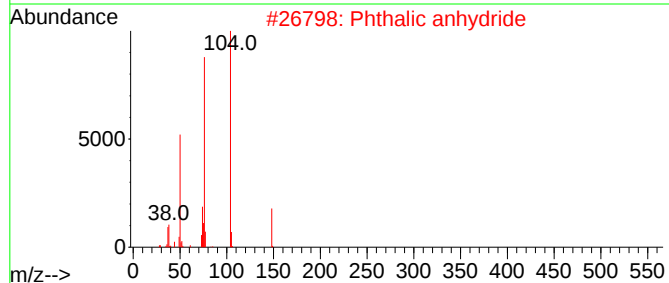
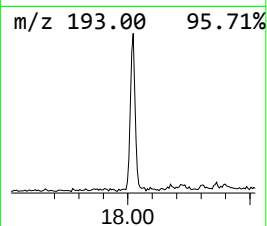
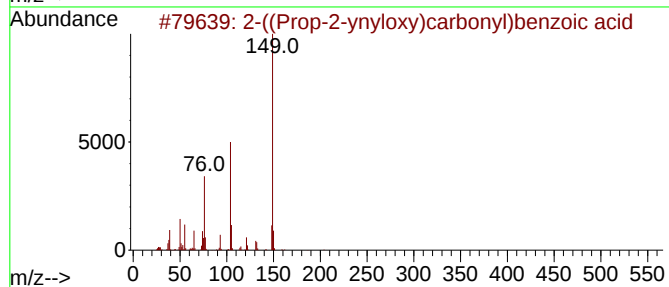
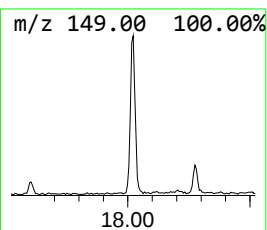
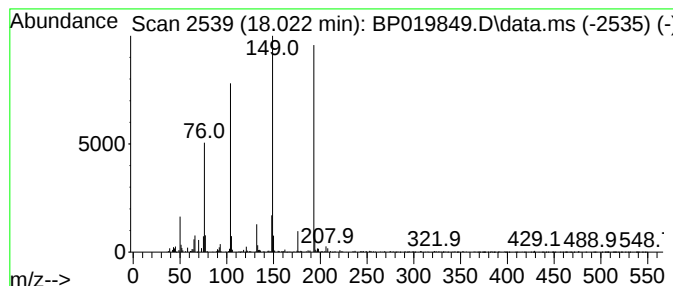
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-((Prop-2-ynyloxy)carbonyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.022	3.16 ng	161329	Phenanthrene-d10	17.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-((Prop-2-ynyloxy)carbonyl)benz...	204	C11H8O4	006139-61-3	50		
2	Phthalic anhydride	148	C8H4O3	000085-44-9	27		
3	1,4-Benzenedicarboxylic acid, bi...	254	C12H14O6	000959-26-2	16		
4	1,2-Benzenedicarboxylic acid	166	C8H6O4	000088-99-3	16		
5	Phthalic acid, di(2-methylallyl)...	274	C16H18O4	1000315-58-3	14		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022324\
Data File : BP019849.D
Acq On : 23 Feb 2024 18:21
Operator : MA/JU
Sample : P1537-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
13

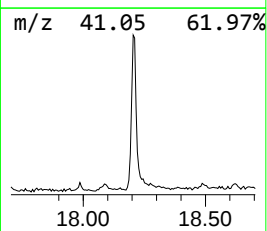
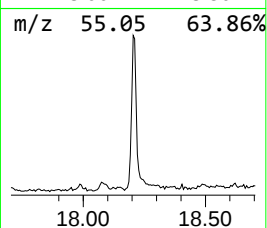
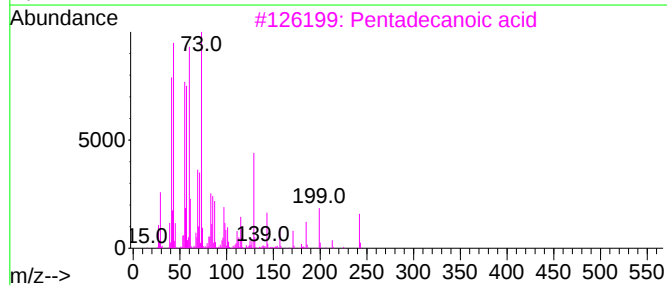
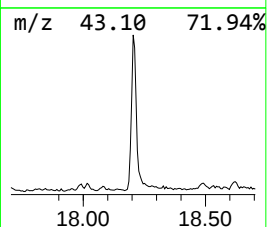
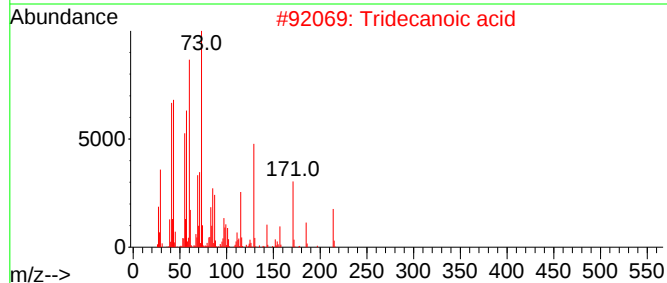
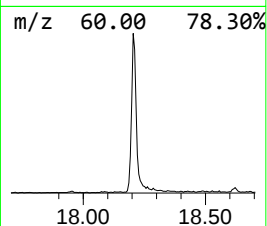
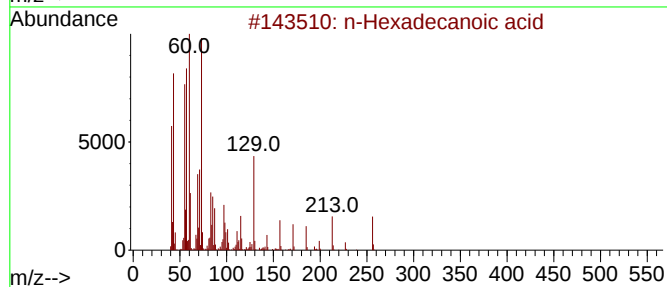
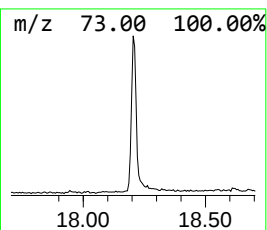
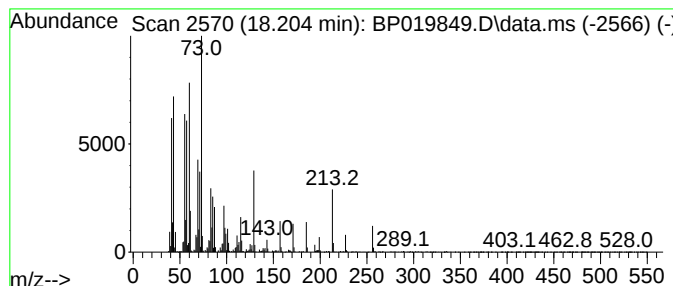
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.204	12.93 ng	660449	Phenanthrene-d10	17.310

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022324\
Data File : BP019849.D
Acq On : 23 Feb 2024 18:21
Operator : MA/JU
Sample : P1537-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
13

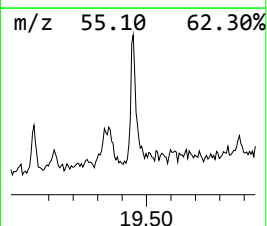
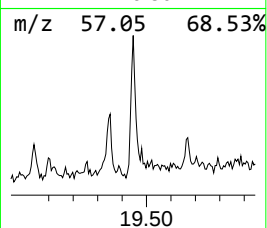
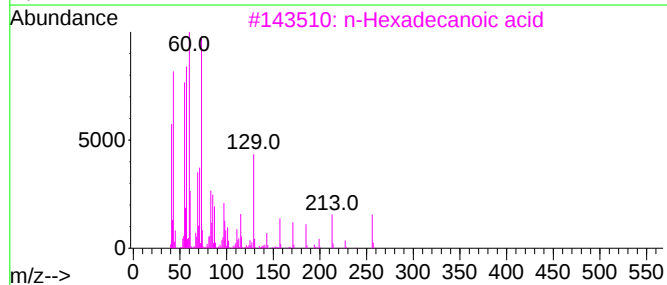
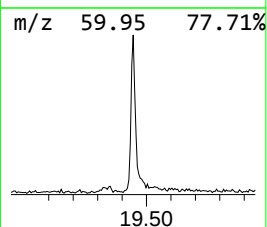
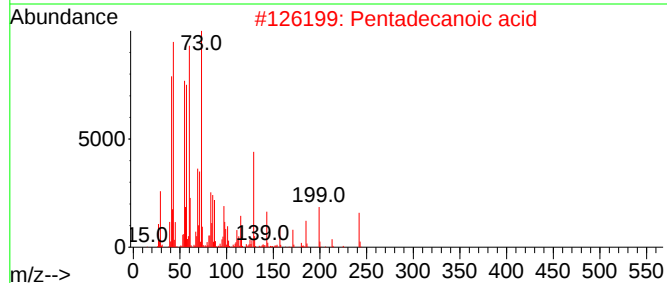
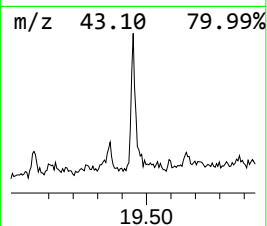
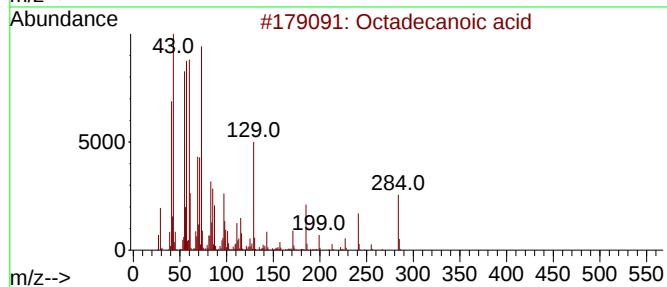
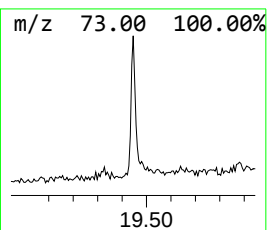
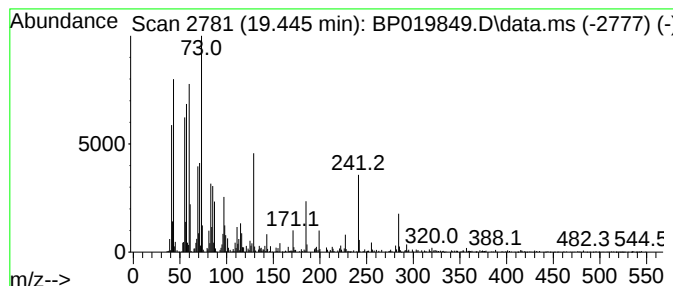
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.445	3.81 ng	243335	Chrysene-d12	21.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	91
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	72
4			Tridecanoic acid	214	C13H26O2	000638-53-9	72
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022324\
Data File : BP019849.D
Acq On : 23 Feb 2024 18:21
Operator : MA/JU
Sample : P1537-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

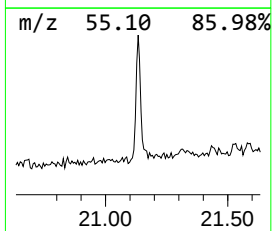
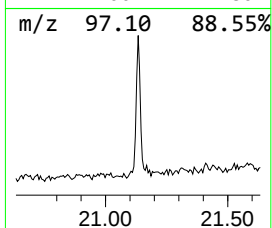
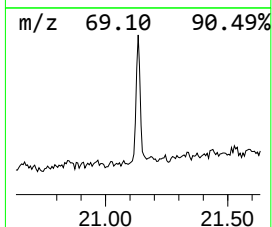
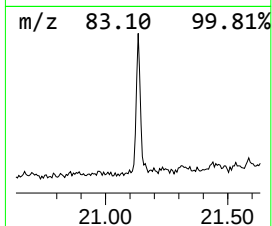
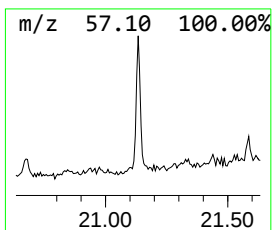
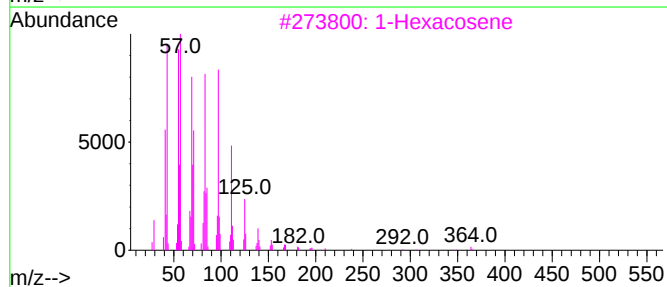
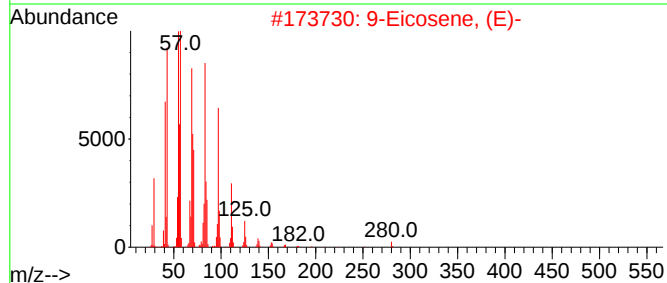
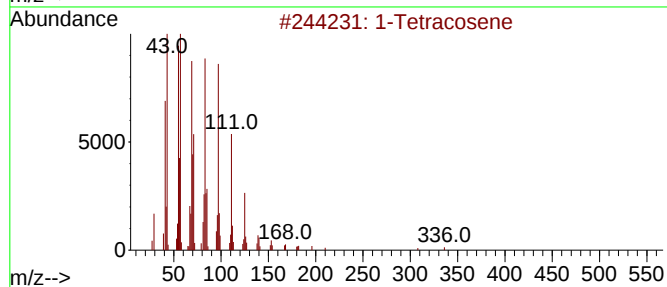
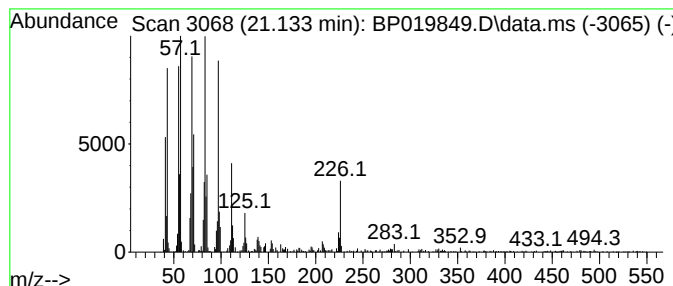
Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Tetracosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.133	5.18 ng	330802	Chrysene-d12	21.416	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tetracosene	336	C24H48	010192-32-2	96
2	9-Eicosene, (E)-	280	C20H40	074685-29-3	93
3	1-Hexacosene	364	C26H52	018835-33-1	93
4	Pentacos-1-ene	350	C25H50	016980-85-1	93
5	Heptacos-1-ene	378	C27H54	015306-27-1	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022324\
Data File : BP019849.D
Acq On : 23 Feb 2024 18:21
Operator : MA/JU
Sample : P1537-13
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.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-...	5.022	16.6	ng	405443	1	7.905	487471	20.0
Hexanoic acid, ...	9.552	8.7	ng	313724	2	10.704	724865	20.0
Phthalic anhydride	12.522	2.1	ng	76676	2	10.704	724865	20.0
2,4,7,9-Tetrame...	13.445	38.4	ng	1611680	3	14.545	840412	20.0
unknown14.769	14.769	4.0	ng	168588	3	14.545	840412	20.0
2-((Prop-2-ynyl...	18.022	3.2	ng	161329	4	17.310	1021710	20.0
n-Hexadecanoic ...	18.204	12.9	ng	660449	4	17.310	1021710	20.0
Octadecanoic acid	19.445	3.8	ng	243335	5	21.416	1276760	20.0
1-Tetracosene	21.133	5.2	ng	330802	5	21.416	1276760	20.0