

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
 Data File : BP019834.D
 Acq On : 22 Feb 2024 20:38
 Operator : MA/JU
 Sample : P1521-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 CG-MW-23-Q

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: BP019834.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.811	278	293	301	rBV	64006	151823	3.04%	0.747%
2	5.017	323	328	338	rVB	80366	120404	2.41%	0.592%
3	5.470	394	405	414	rBV	540642	834218	16.70%	4.105%
4	6.128	513	517	531	rVB	39704	76378	1.53%	0.376%
5	7.069	670	677	689	rBV	285490	488172	9.77%	2.402%
6	7.893	810	817	824	rBV	248959	399577	8.00%	1.966%
7	9.063	1008	1016	1032	rBV	747596	1311750	26.26%	6.455%
8	10.110	1188	1194	1207	rBV5	24123	57178	1.14%	0.281%
9	10.693	1285	1293	1301	rBV	282566	486321	9.74%	2.393%
10	12.346	1568	1574	1585	rBV2	24449	56254	1.13%	0.277%
11	13.157	1703	1712	1725	rBV	1996943	3132089	62.70%	15.412%
12	14.363	1909	1917	1926	rVB3	29186	67939	1.36%	0.334%
13	14.528	1939	1945	1954	rBV	443260	682831	13.67%	3.360%
14	16.028	2193	2200	2209	rBV	1977493	2895911	57.97%	14.250%
15	16.240	2232	2236	2249	rVB3	21139	60210	1.21%	0.296%
16	17.287	2407	2414	2421	rBV	566845	869342	17.40%	4.278%
17	18.187	2562	2567	2575	rBV	319506	460947	9.23%	2.268%
18	19.422	2773	2777	2786	rBV	110780	164135	3.29%	0.808%
19	19.857	2845	2851	2861	rBV	4147295	4995244	100.00%	24.581%
20	20.163	2901	2903	2907	rVB3	62900	58176	1.16%	0.286%
21	20.651	2982	2986	2990	rBV2	107254	149521	2.99%	0.736%
22	21.104	3060	3063	3068	rVB	279626	328568	6.58%	1.617%
23	21.386	3106	3111	3118	rBV	746564	1029285	20.61%	5.065%
24	23.098	3398	3402	3407	rVB	231014	377042	7.55%	1.855%
25	23.804	3517	3522	3531	rVB	516923	1068475	21.39%	5.258%

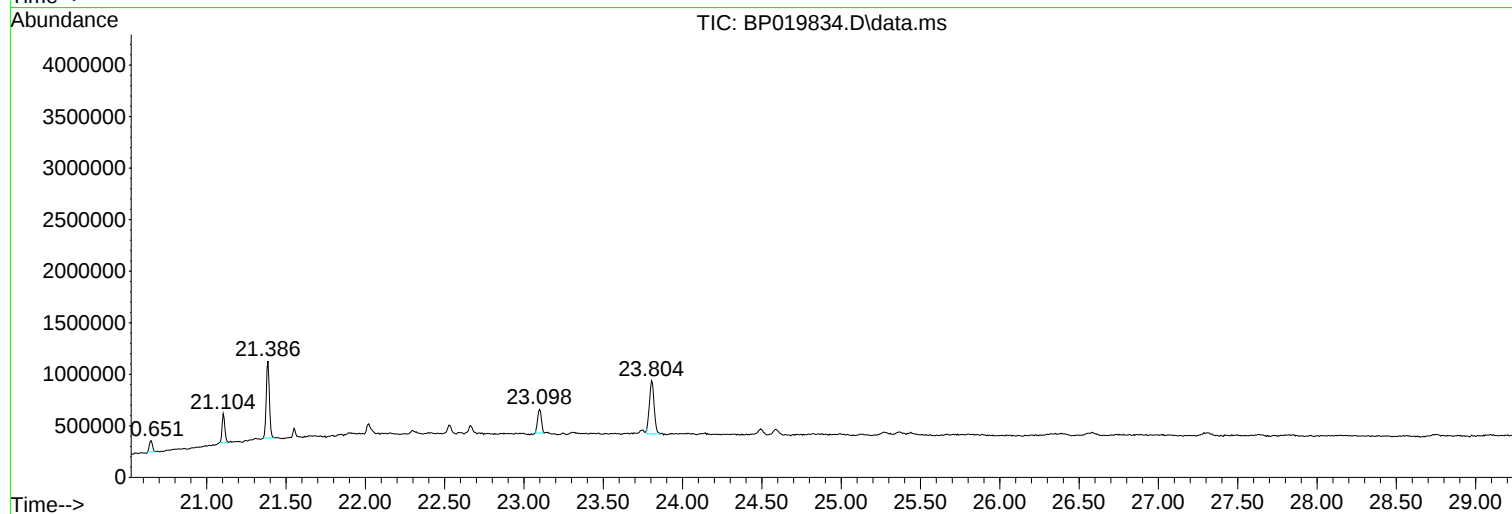
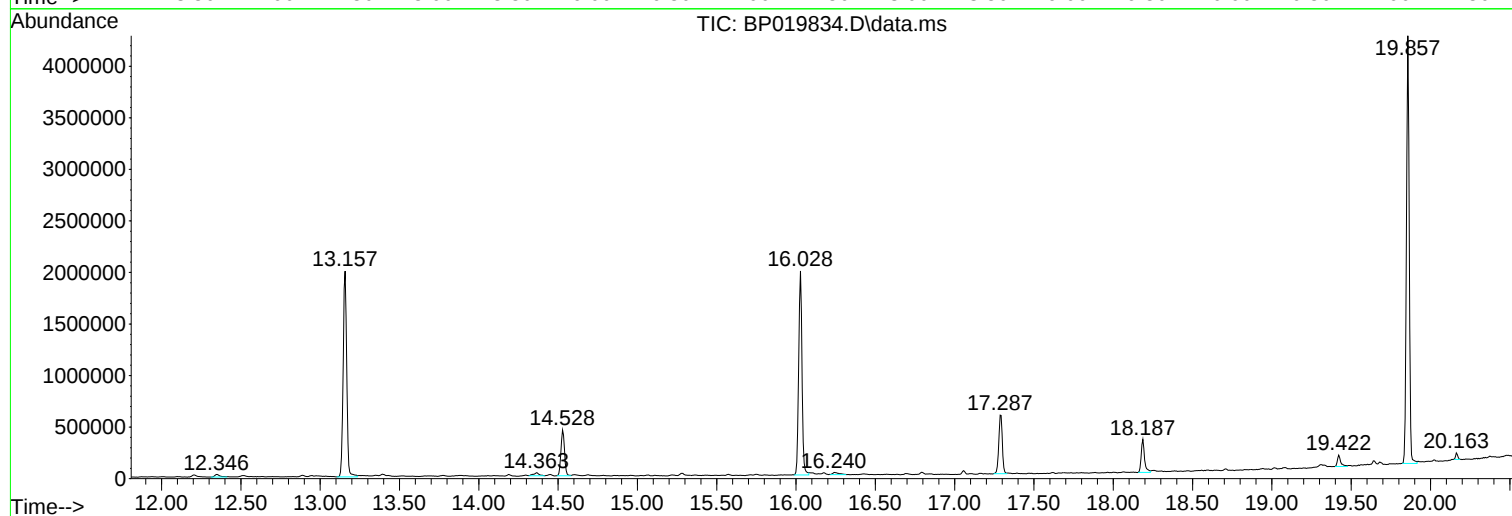
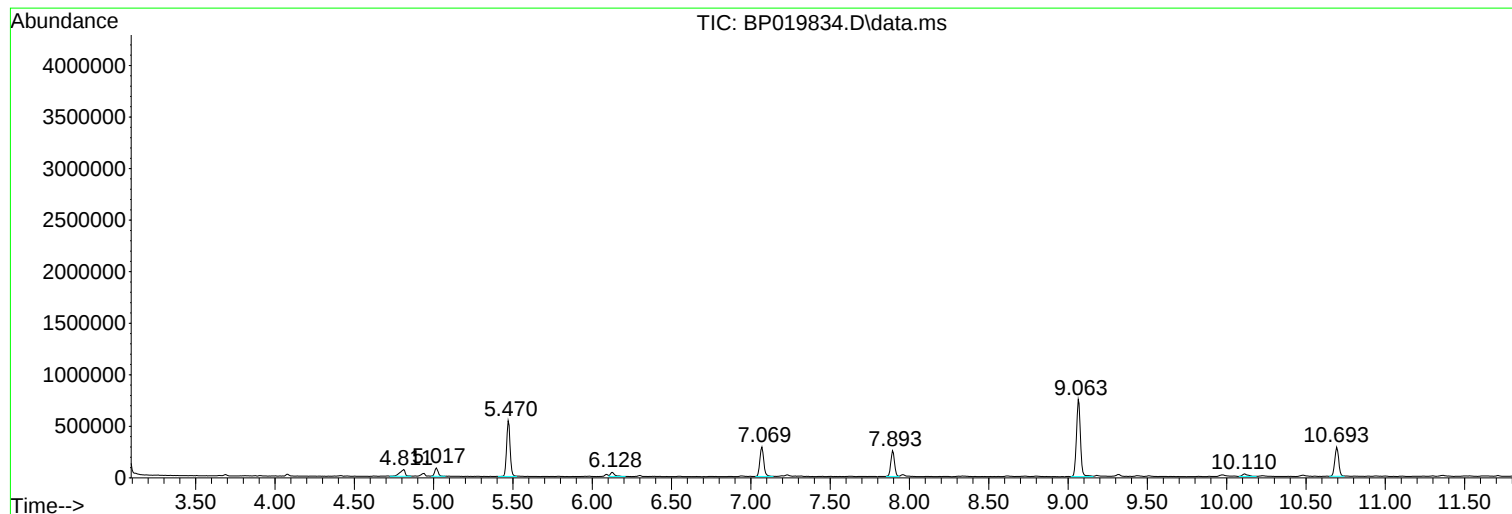
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP013124.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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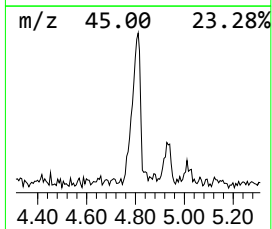
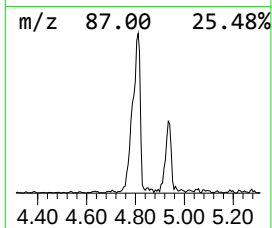
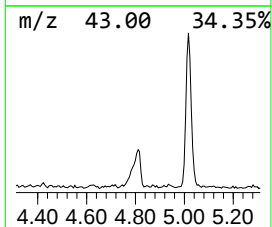
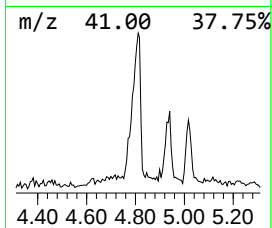
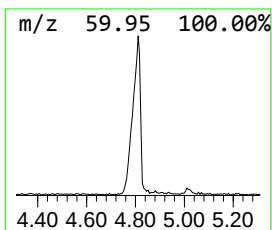
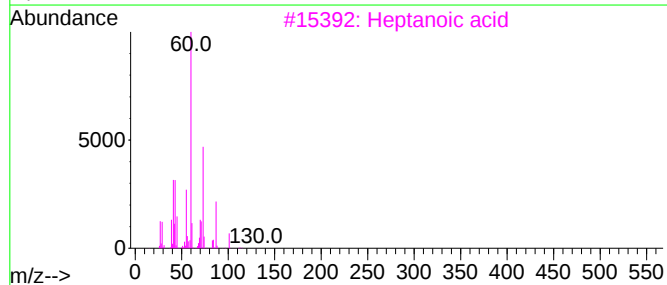
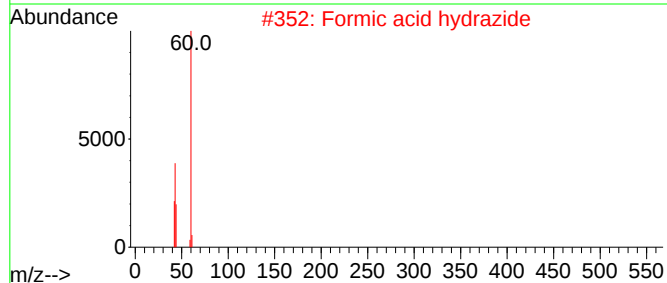
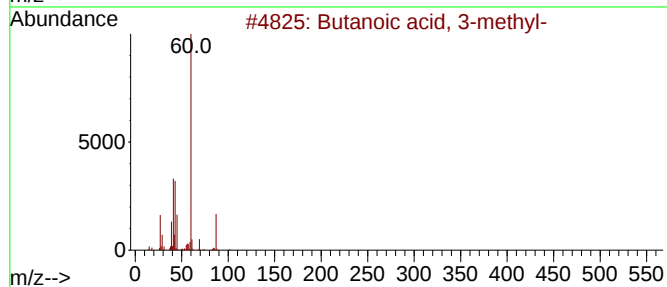
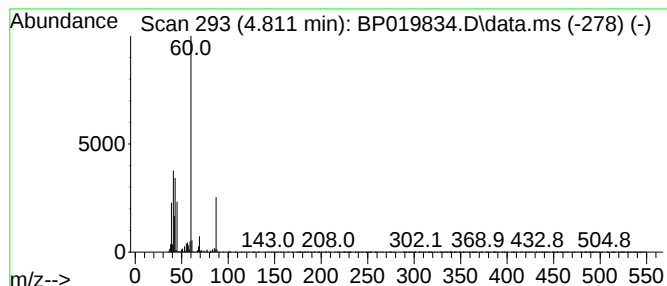
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butanoic acid, 3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.811	7.60 ng	151823	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
2			Formic acid hydrazide	60	CH4N2O	000624-84-0	50
3			Heptanoic acid	130	C7H14O2	000111-14-8	40
4			Butanoic acid, 4-chloro-	122	C4H7ClO2	000627-00-9	39
5			Pentanoic acid	102	C5H10O2	000109-52-4	33



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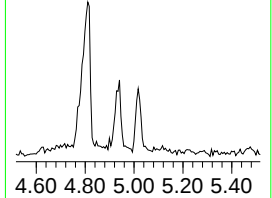
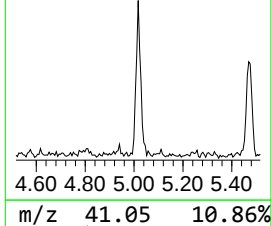
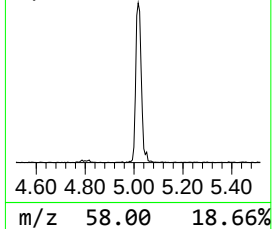
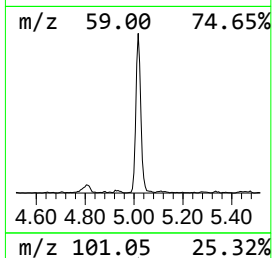
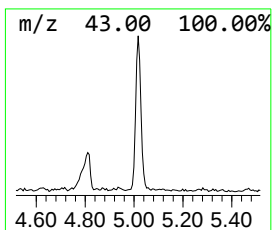
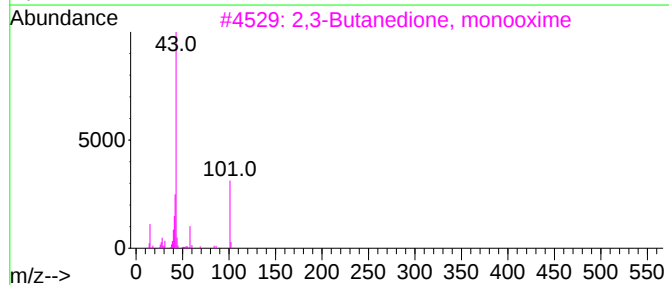
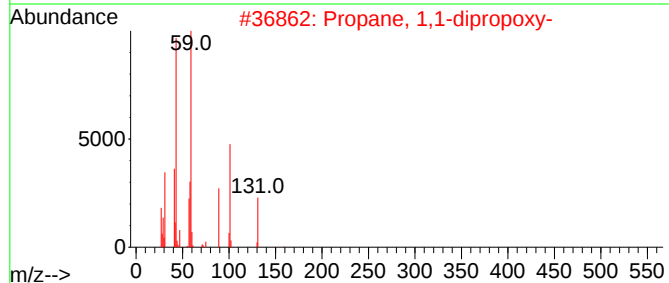
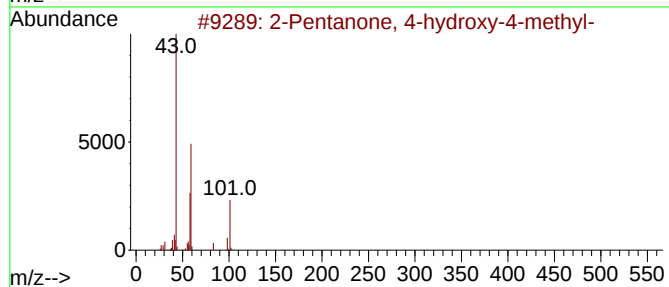
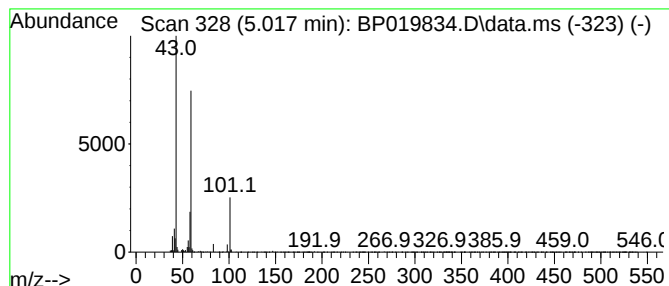
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.017	6.03 ng	120404	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Propane, 1,1-dipropoxy-	160	C9H20O2	004744-11-0	39
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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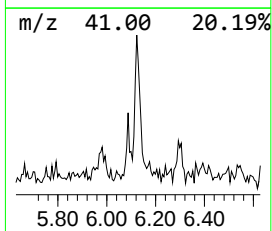
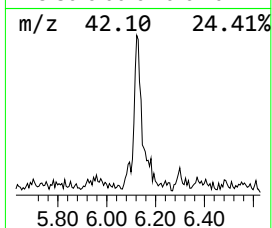
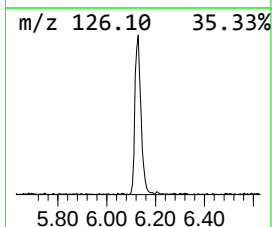
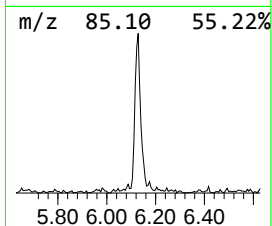
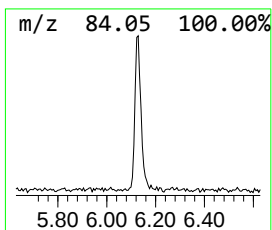
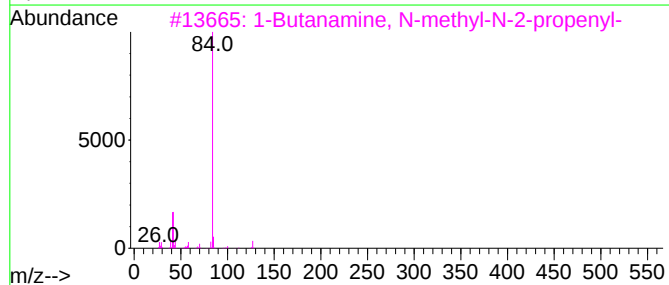
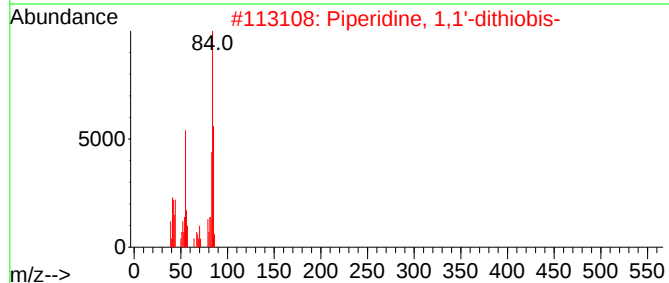
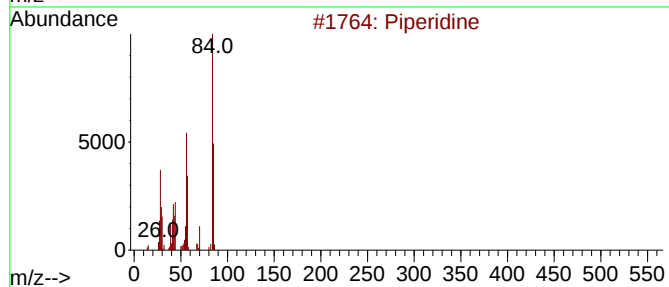
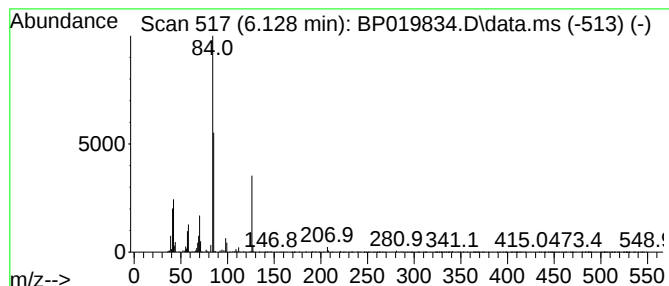
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Peak Number 3 Piperidine Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.128	3.82 ng	76378	1,4-Dichlorobenzene-d4	7.893

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Piperidine	85	C5H11N	000110-89-4	59
2			Piperidine, 1,1'-dithiobis-	232	C10H20N2S2	010220-20-9	50
3			1-Butanamine, N-methyl-N-2-prope...	127	C8H17N	024209-62-9	43
4			Cyclohexanone, 2-(dimethylamino)-	141	C8H15NO	006970-60-1	40
5			Trimethylsilyl cyanide	99	C4H9NSi	007677-24-9	38



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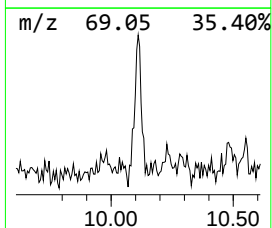
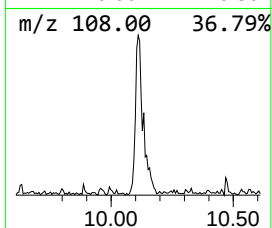
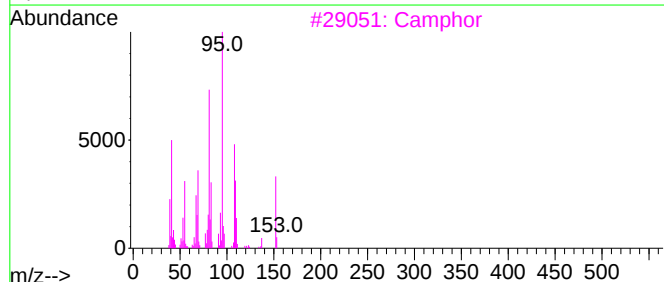
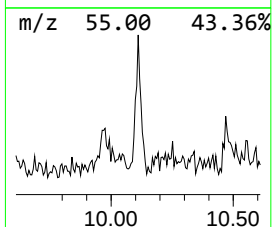
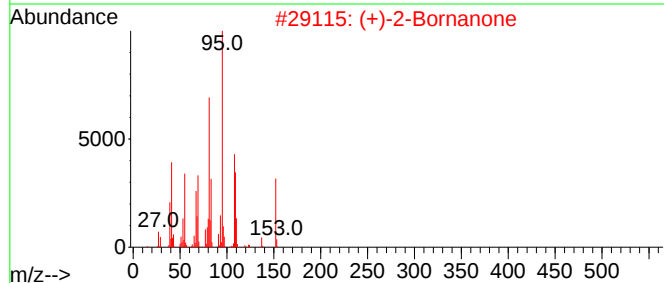
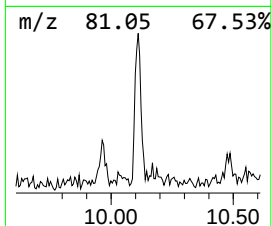
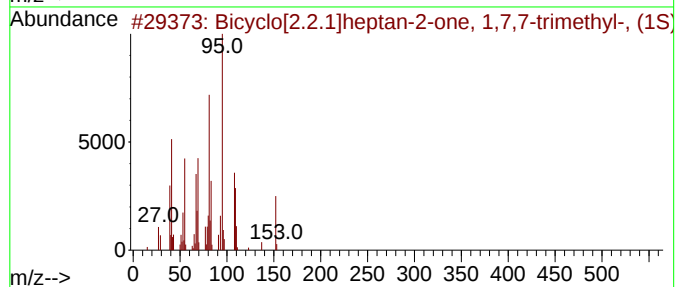
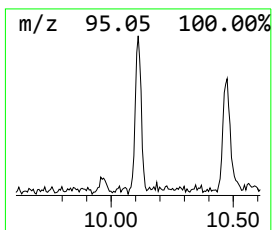
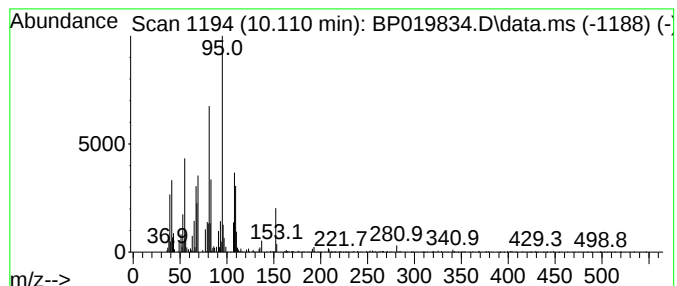
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Peak Number 4 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.111	2.35 ng	57178	Naphthalene-d8	10.693

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	98
2			(+)-2-Bornanone	152	C10H16O	000464-49-3	97
3			Camphor	152	C10H16O	000076-22-2	96
4			Tricyclo[2.2.1.0(2,6)]heptan-3-o...	152	C10H16O	062560-53-6	58
5			5,7-Octadien-4-one, 2,6-dimethyl...	152	C10H16O	006752-80-3	49



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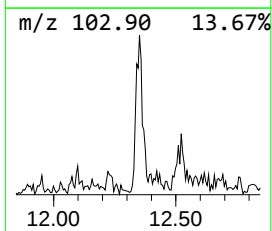
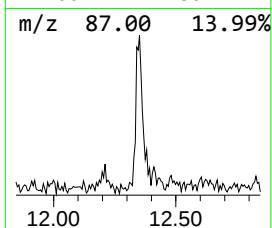
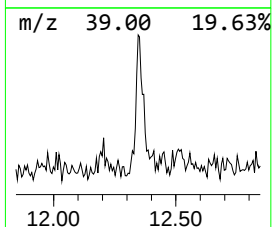
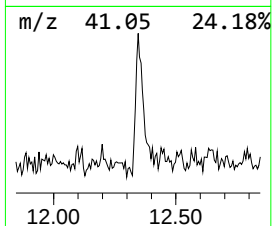
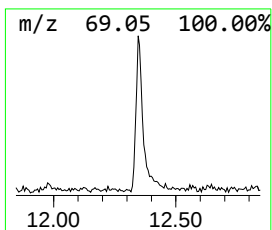
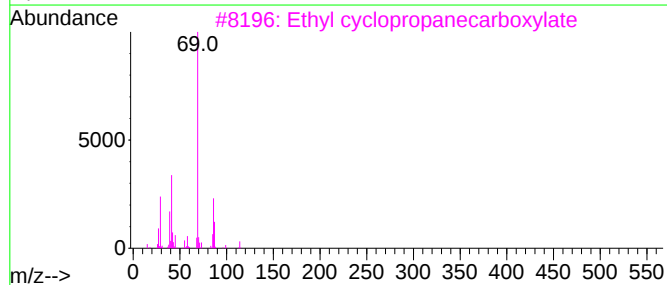
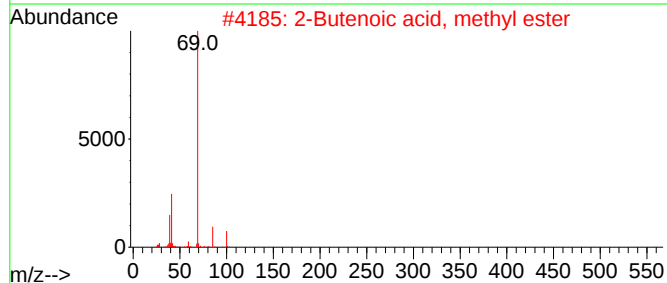
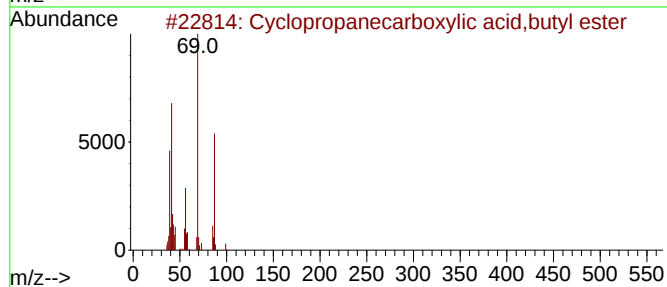
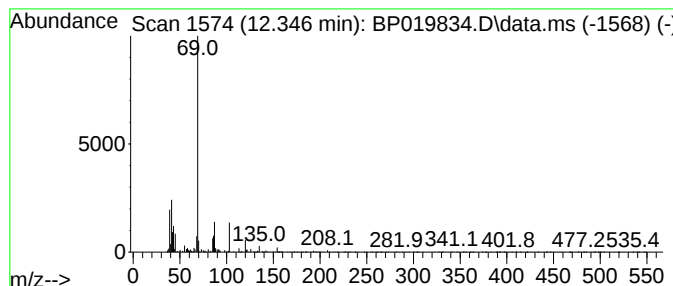
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Peak Number 5 Cyclopropanecarboxylic acid... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.346	2.31 ng	56254	Naphthalene-d8	10.693

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	64
2			2-Butenoic acid, methyl ester	100	C5H8O2	018707-60-3	52
3			Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	50
4			Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	40
5			(E)-2-Methylbut-2-en-1-yl methac...	154	C9H14O2	088142-95-4	40



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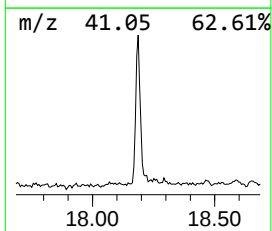
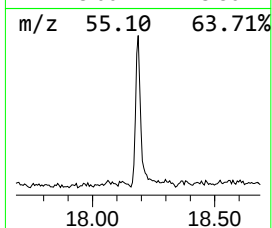
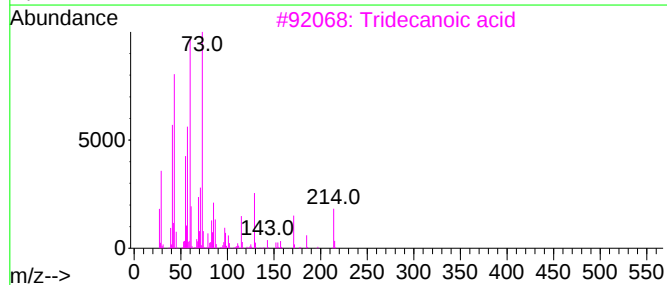
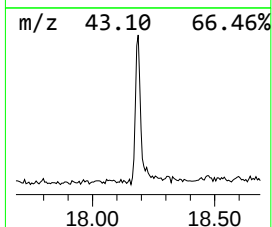
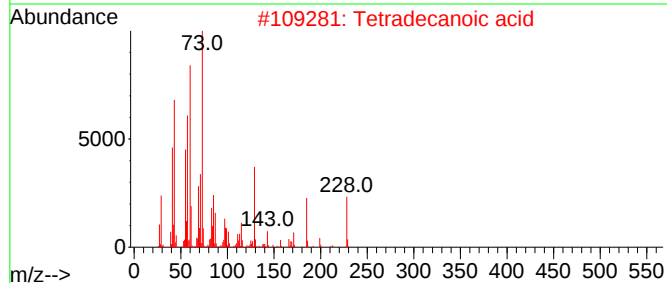
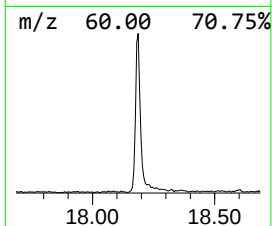
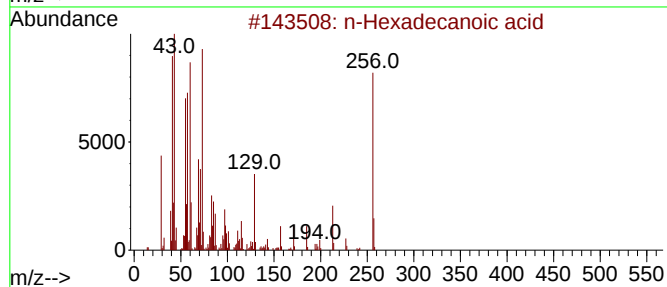
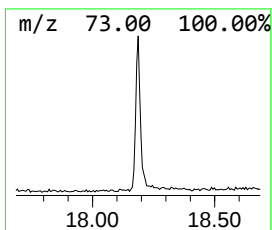
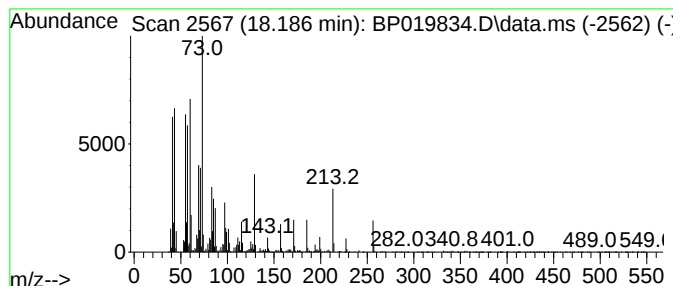
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.186	10.60 ng	460947	Phenanthrene-d10	17.287

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3			Tridecanoic acid	214	C13H26O2	000638-53-9	86
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	74
5			Octadecanoic acid	284	C18H36O2	000057-11-4	62



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019834.D
Acq On : 22 Feb 2024 20:38
Operator : MA/JU
Sample : P1521-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23-Q

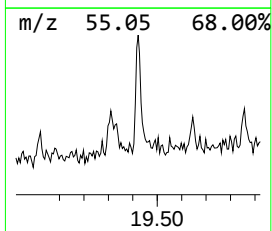
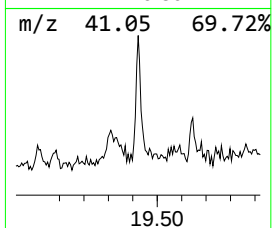
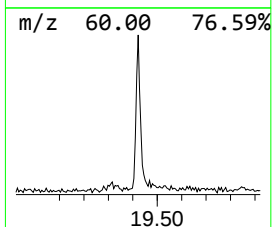
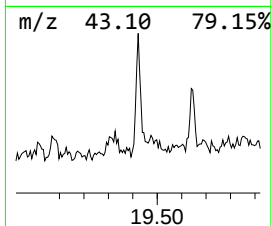
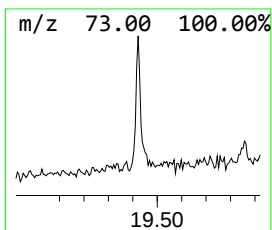
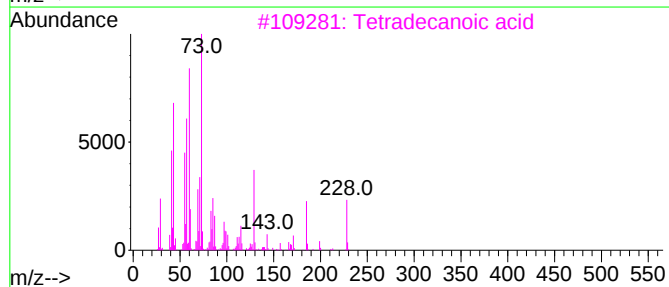
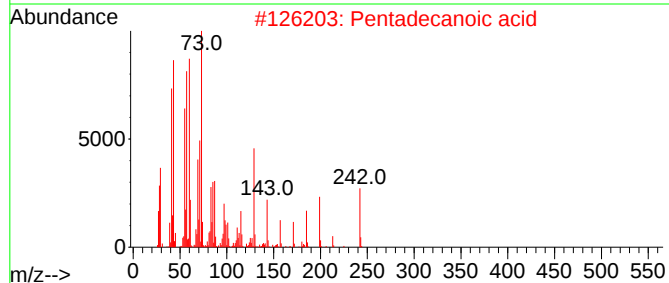
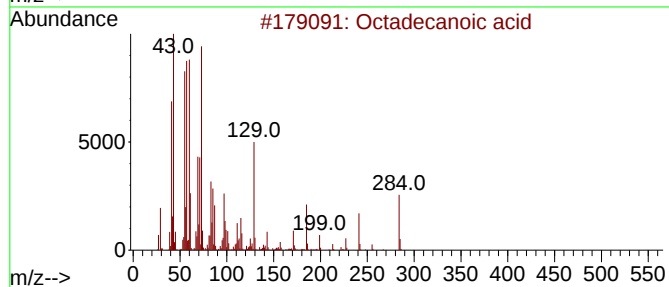
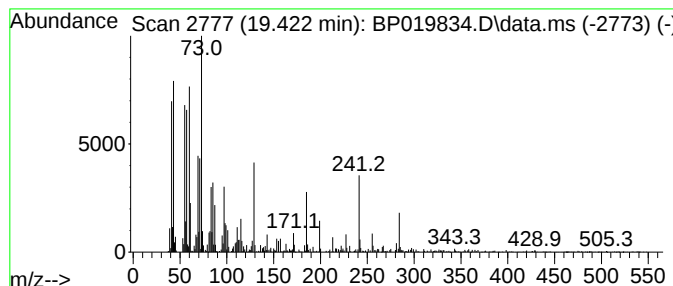
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.422	3.19 ng	164135	Chrysene-d12	21.386

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	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4			n-Decanoic acid	172	C10H20O2	000334-48-5	70
5			Heneicosanoic acid	326	C21H42O2	002363-71-5	60



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019834.D
Acq On : 22 Feb 2024 20:38
Operator : MA/JU
Sample : P1521-02
Misc :
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Instrument :
BNA_P
ClientSampleId :
CG-MW-23-Q

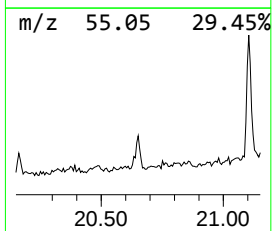
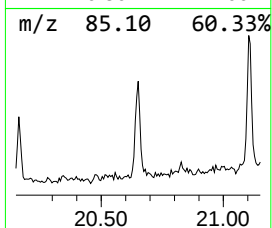
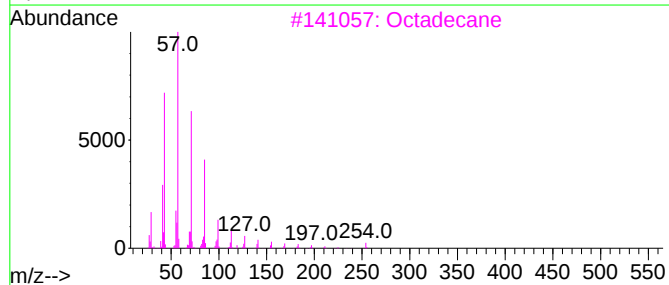
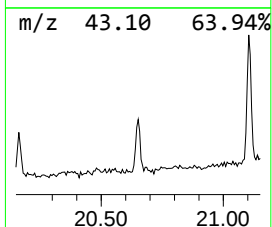
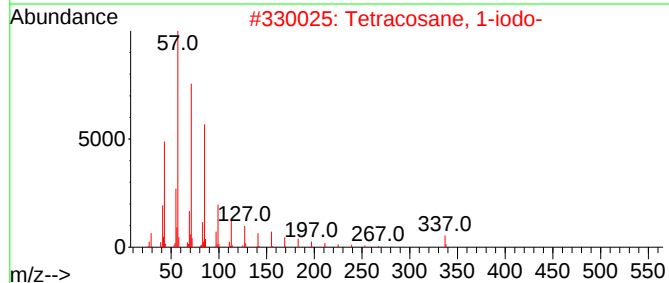
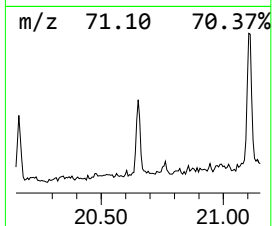
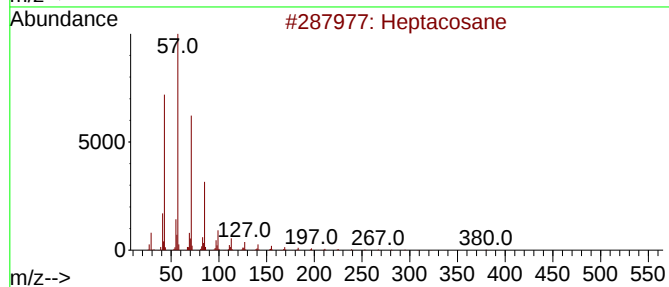
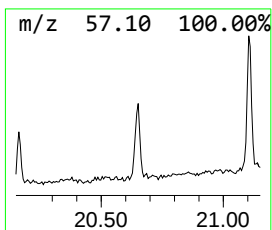
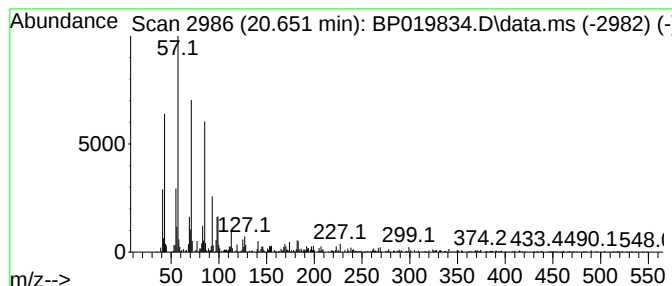
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Heptacosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.651	2.91 ng	149521	Chrysene-d12	21.386

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptacosane	380	C27H56	000593-49-7	92
2		Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87
3		Octadecane	254	C18H38	000593-45-3	87
4		Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5		Heptadecane	240	C17H36	000629-78-7	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019834.D
Acq On : 22 Feb 2024 20:38
Operator : MA/JU
Sample : P1521-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23-Q

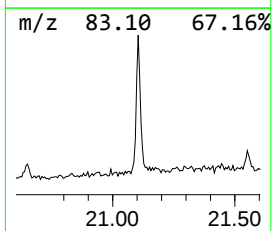
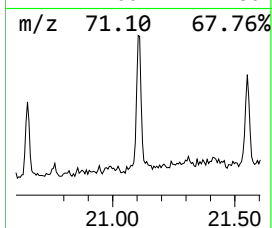
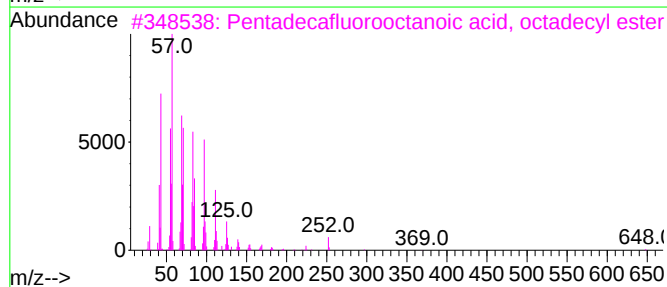
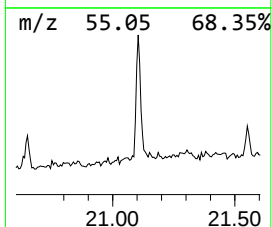
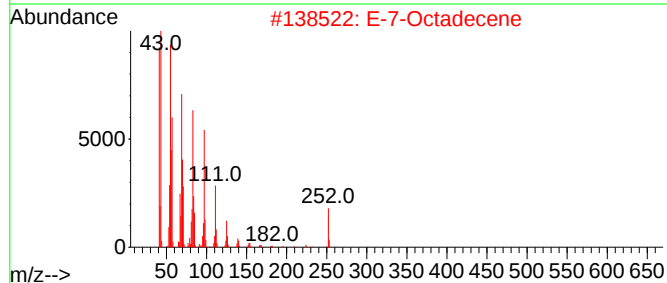
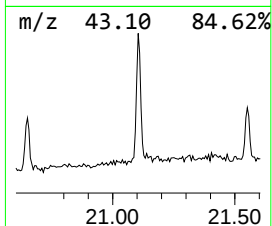
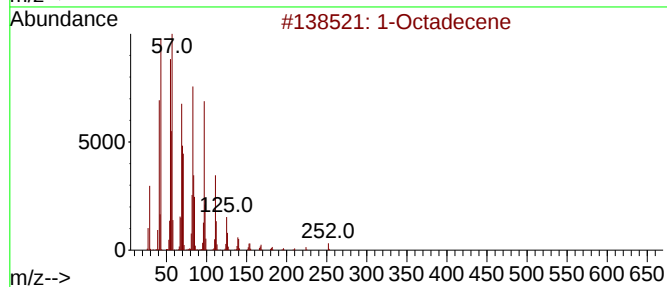
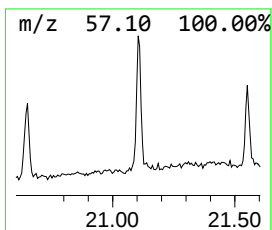
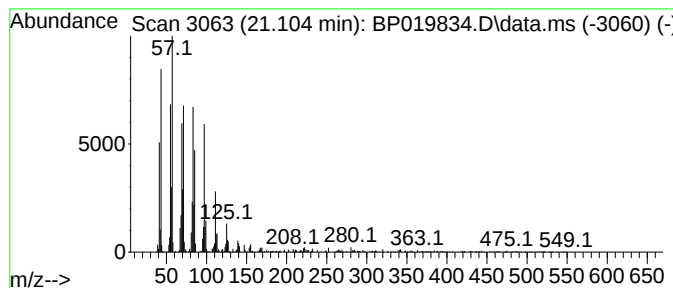
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Octadecene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.104	6.38 ng	328568	Chrysene-d12	21.386

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octadecene			252	C18H36	000112-88-9	95
2	E-7-Octadecene			252	C18H36	1000130-92-0	92
3	Pentadecafluorooctanoic acid, oc...			666	C26H37F15O2	1000406-04-8	91
4	Oxalic acid, isobutyl hexadecyl ...			370	C22H42O4	1000309-38-1	91
5	Oxalic acid, hexadecyl propyl ester			356	C21H40O4	1000309-26-9	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019834.D
Acq On : 22 Feb 2024 20:38
Operator : MA/JU
Sample : P1521-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
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ClientSampleId :
CG-MW-23-Q

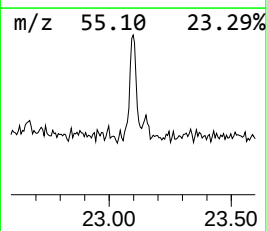
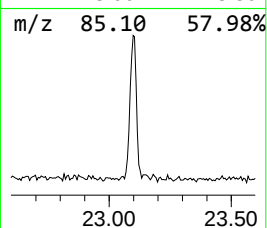
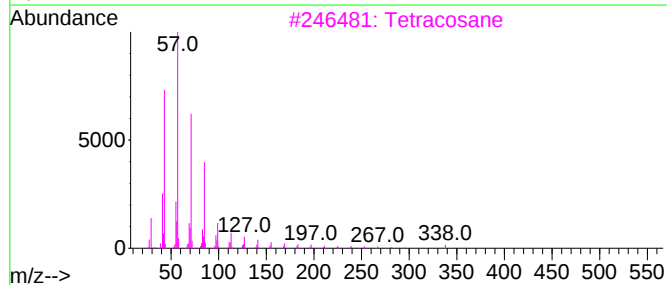
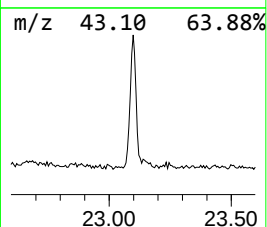
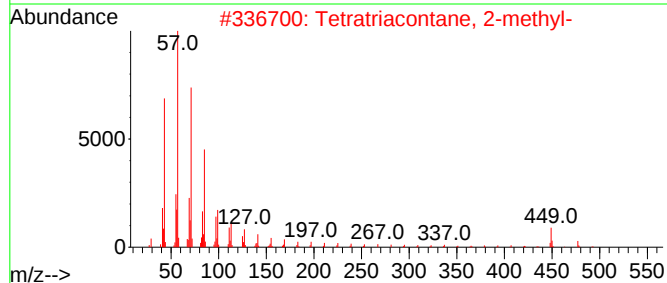
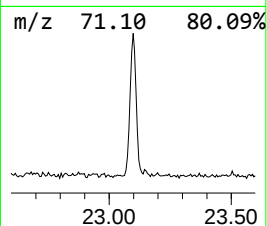
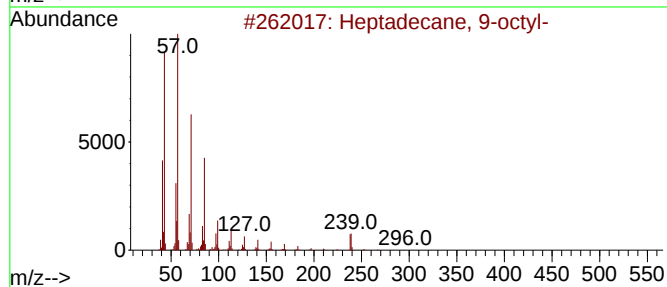
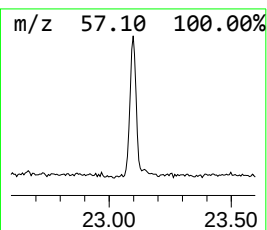
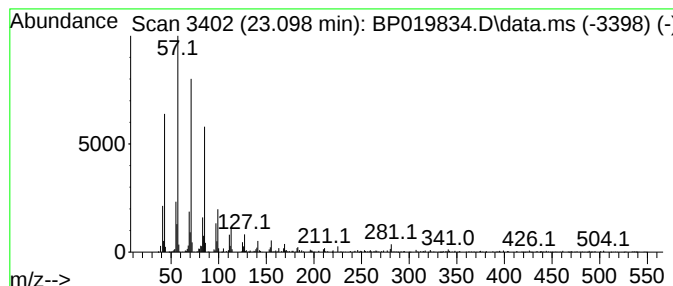
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Heptadecane, 9-octyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.098	7.06 ng	377042	Perylene-d12	23.804

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
2		Tetratriacontane, 2-methyl-	493	C35H72	014167-65-8	93
3		Tetracosane	338	C24H50	000646-31-1	93
4		Octadecane, 2-methyl-	268	C19H40	001560-88-9	93
5		Octacosane, 2-methyl-	408	C29H60	001560-98-1	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP022224\
Data File : BP019834.D
Acq On : 22 Feb 2024 20:38
Operator : MA/JU
Sample : P1521-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
CG-MW-23-Q

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
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2-Pentanone, 4-...	5.017	6.0	ng	120404	1	7.893	399577	20.0
Piperidine	6.128	3.8	ng	76378	1	7.893	399577	20.0
Bicyclo[2.2.1]h...	10.111	2.4	ng	57178	2	10.693	486321	20.0
Cyclopropanecar...	12.346	2.3	ng	56254	2	10.693	486321	20.0
n-Hexadecanoic ...	18.186	10.6	ng	460947	4	17.287	869342	20.0
Octadecanoic acid	19.422	3.2	ng	164135	5	21.386	1029290	20.0
Heptacosane	20.651	2.9	ng	149521	5	21.386	1029290	20.0
1-Octadecene	21.104	6.4	ng	328568	5	21.386	1029290	20.0
Heptadecane, 9-...	23.098	7.1	ng	377042	6	23.804	1068480	20.0