

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
 Data File : BP021519.D
 Acq On : 15 Aug 2024 18:37
 Operator : RC/JU
 Sample : P3582-02
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-855-J-SO-1.5-2-081224

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-BP081324.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP021519.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	25	rVB	4645849	5839191	39.40%	5.497%
2	3.540	89	94	105	rBV	440787	571740	3.86%	0.538%
3	4.934	325	331	338	rVB	307029	419386	2.83%	0.395%
4	5.393	402	409	420	rBV	6268436	8879057	59.91%	8.359%
5	6.957	666	675	686	rBV	5687198	9194720	62.04%	8.656%
6	7.799	812	818	825	rBV	1633205	2633281	17.77%	2.479%
7	8.116	865	872	882	rBV3	84580	153957	1.04%	0.145%
8	8.946	1005	1013	1022	rBV	3311697	5525214	37.28%	5.202%
9	9.504	1101	1108	1114	rBV	131177	207459	1.40%	0.195%
10	10.587	1284	1292	1300	rBV	2032740	3540860	23.89%	3.334%
11	11.322	1410	1417	1428	rBV	467101	814265	5.49%	0.767%
12	13.051	1704	1711	1721	rBV	8029510	11350882	76.59%	10.686%
13	14.439	1940	1947	1954	rVB	3239256	4450465	30.03%	4.190%
14	14.675	1977	1987	1999	rBV3	175314	435179	2.94%	0.410%
15	15.951	2197	2204	2213	rBV	6204357	8532320	57.57%	8.033%
16	17.245	2417	2424	2430	rBV	3369410	5081113	34.29%	4.784%
17	18.192	2577	2585	2595	rBV	1988136	3143700	21.21%	2.960%
18	19.369	2780	2785	2788	rBV	295282	455561	3.07%	0.429%
19	19.522	2805	2811	2832	rVV	2416765	3971769	26.80%	3.739%
20	19.674	2833	2837	2843	rVV	311588	541964	3.66%	0.510%
21	19.739	2845	2848	2852	rVV	233552	340619	2.30%	0.321%
22	19.804	2856	2859	2865	rVB2	130055	169553	1.14%	0.160%
23	19.963	2880	2886	2891	rBV	12504825	14820208	100.00%	13.953%
24	20.769	3020	3023	3028	rBV	213507	251861	1.70%	0.237%
25	21.368	3120	3125	3140	rVB	735394	1386888	9.36%	1.306%
26	21.627	3165	3169	3172	rBV	141859	197715	1.33%	0.186%
27	21.686	3172	3179	3185	rVV2	3028725	5225380	35.26%	4.919%
28	22.651	3338	3343	3353	rBV	277052	564893	3.81%	0.532%
29	23.910	3550	3557	3567	rVB	928804	2242333	15.13%	2.111%
30	25.080	3746	3756	3773	rVB	1811708	5277290	35.61%	4.968%

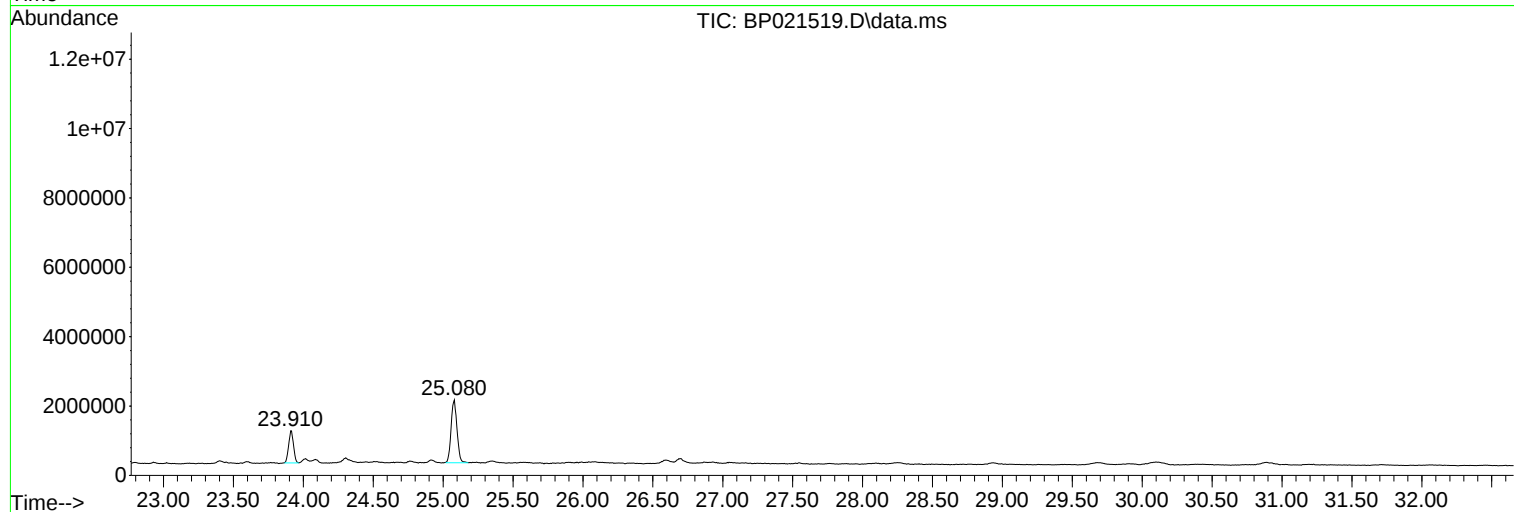
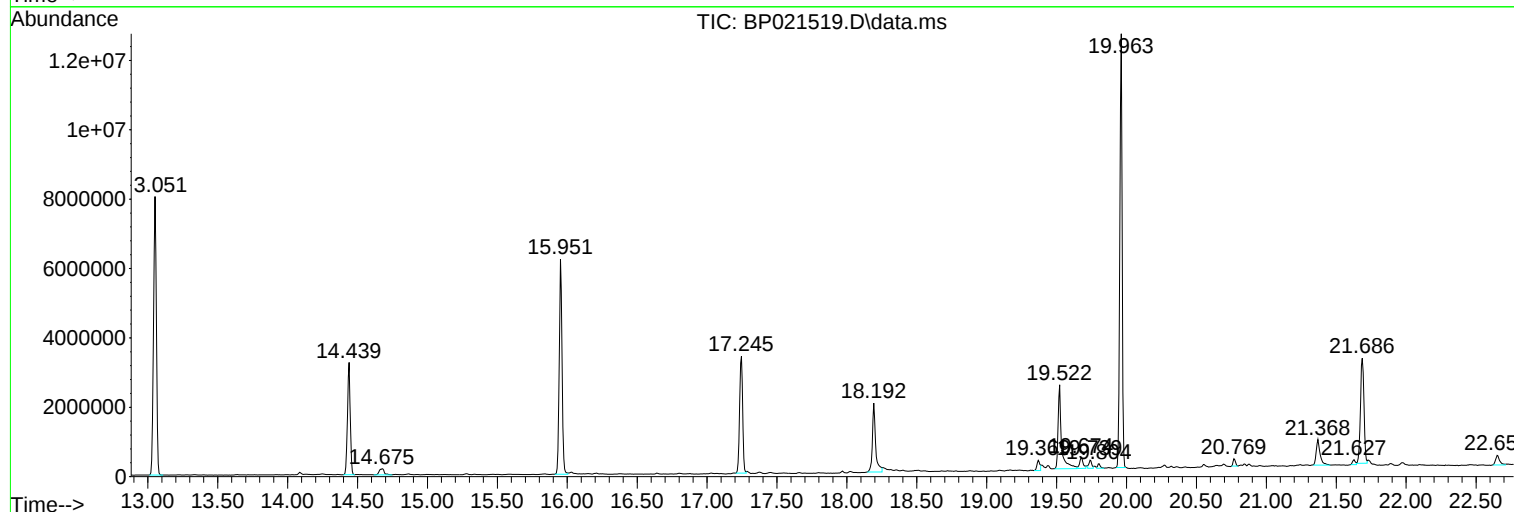
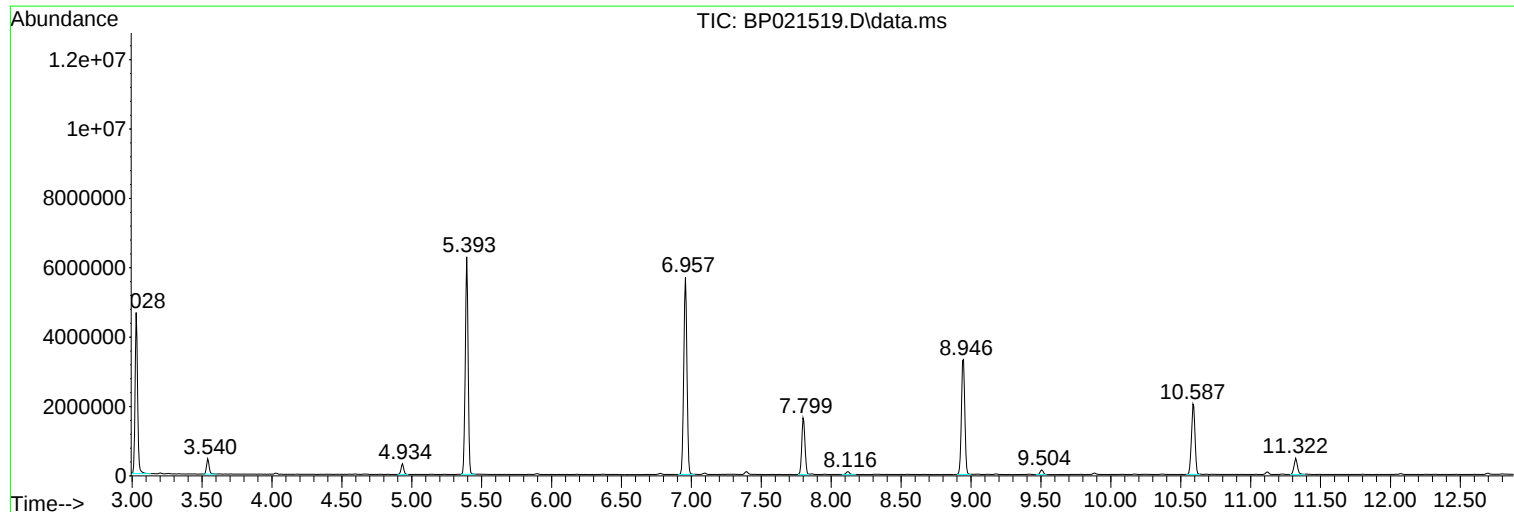
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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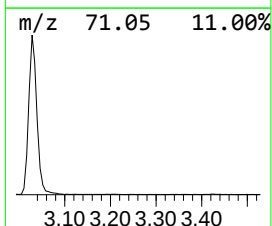
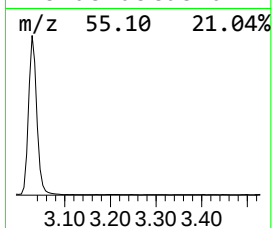
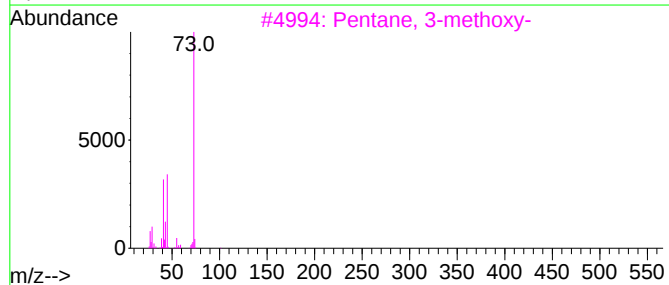
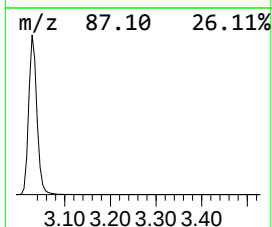
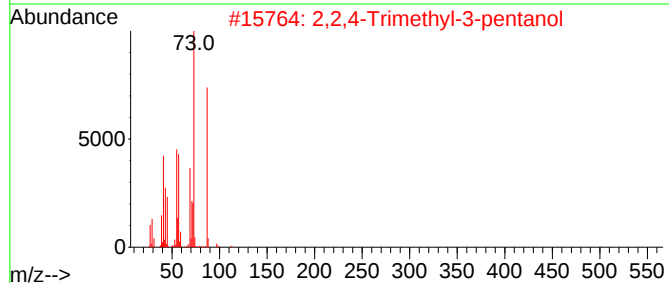
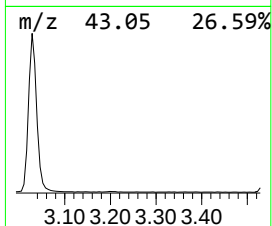
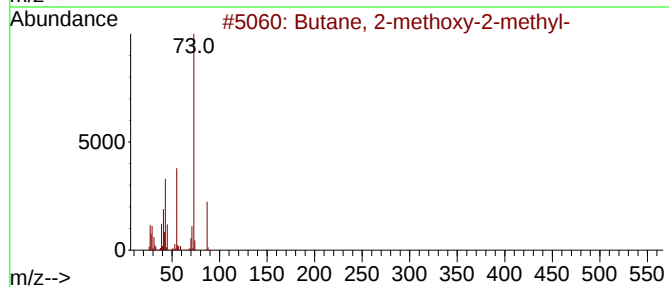
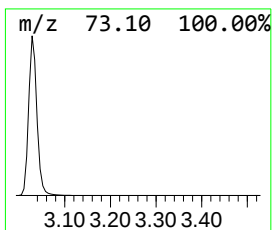
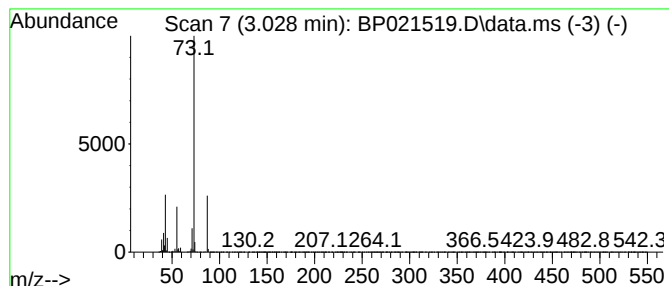
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.028	44.35 ng	5839190	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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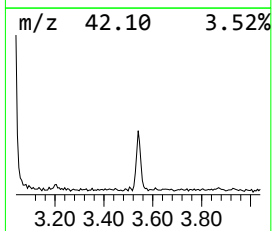
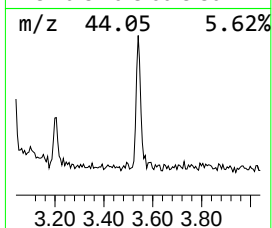
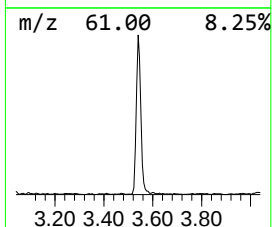
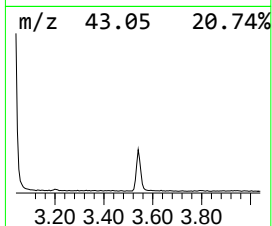
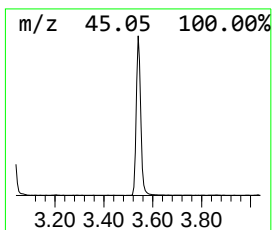
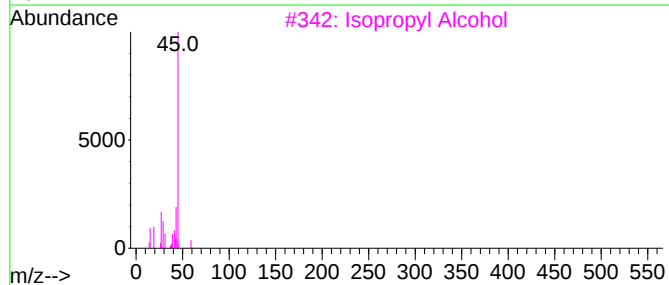
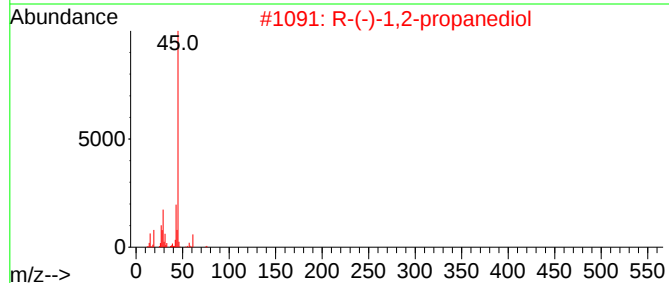
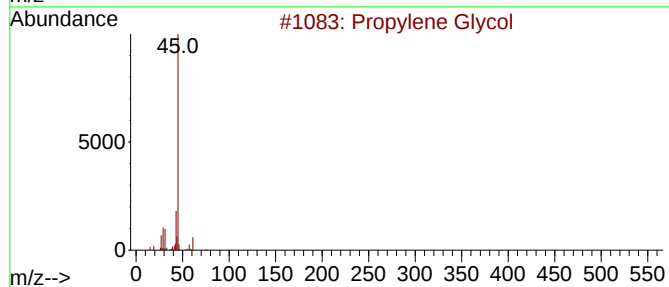
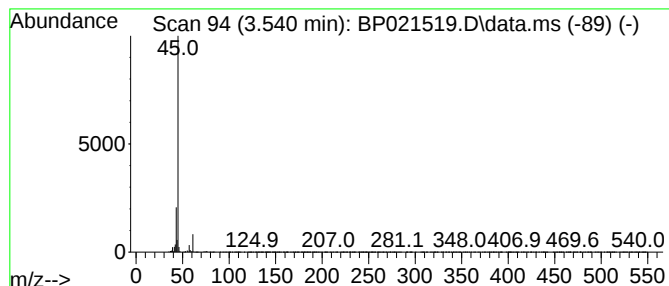
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.540	4.34 ng	571740	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
5			Propane, 2-ethoxy-	88	C5H12O	000625-54-7	9



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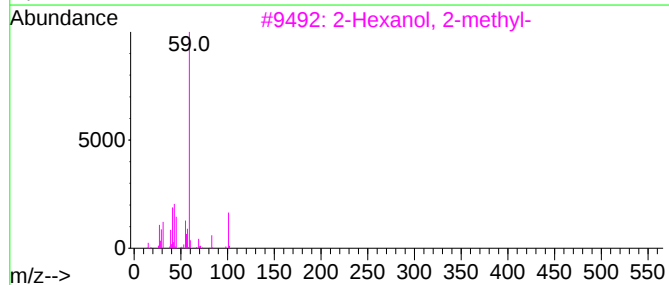
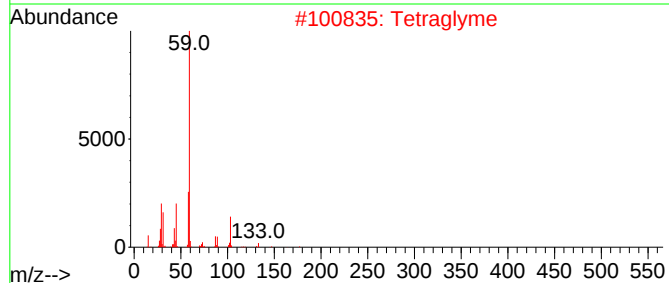
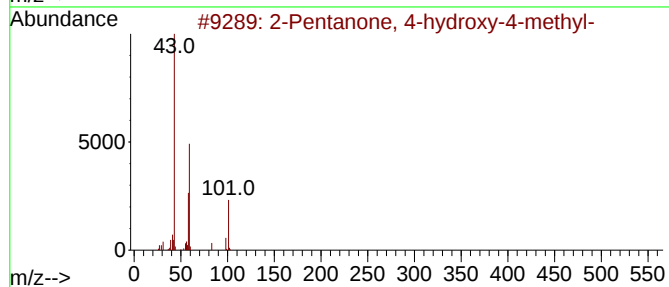
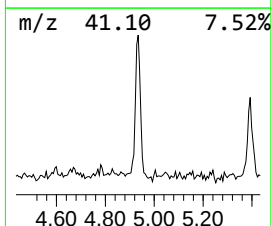
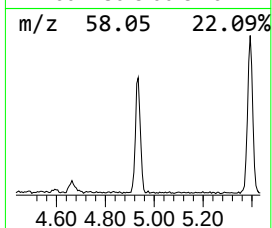
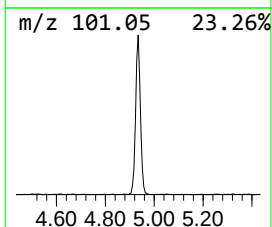
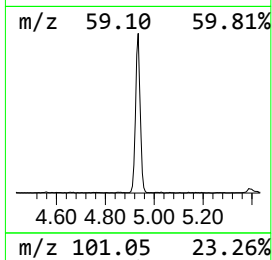
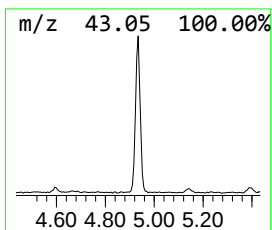
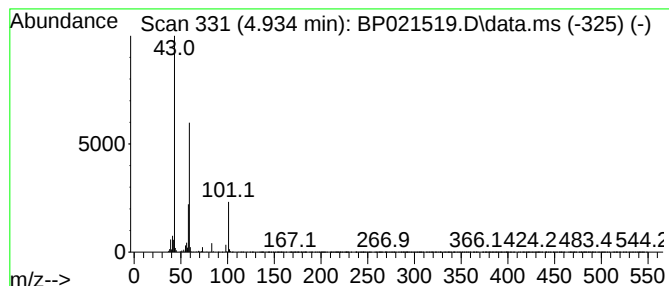
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.934	3.19 ng	419386	1,4-Dichlorobenzene-d4	7.799

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50		
2	Tetraglyme	222	C10H22O5	000143-24-8	28		
3	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25		
4	Hexanamide	115	C6H13NO	000628-02-4	22		
5	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	12		



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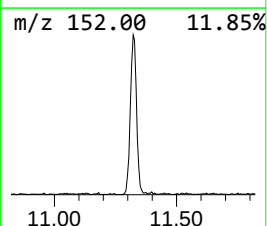
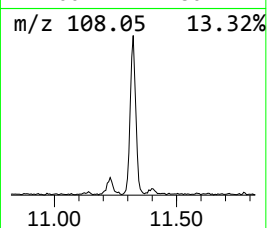
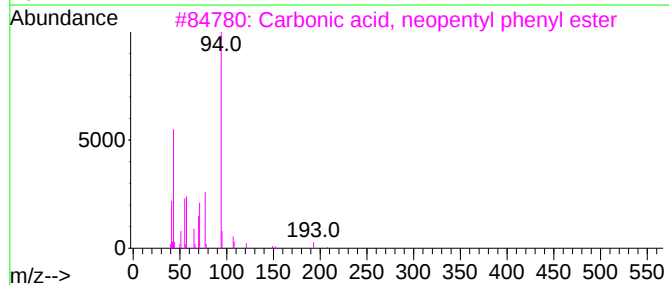
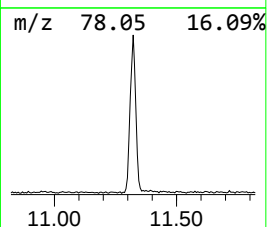
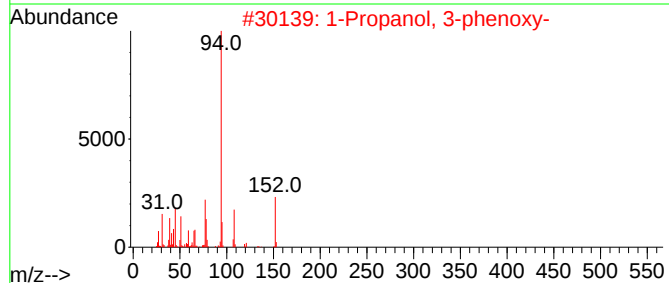
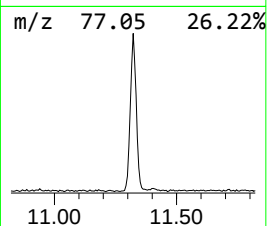
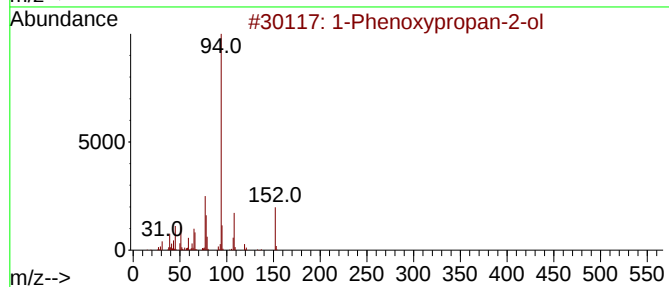
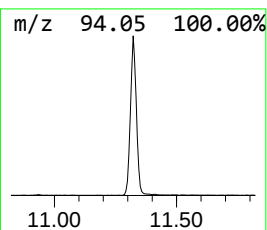
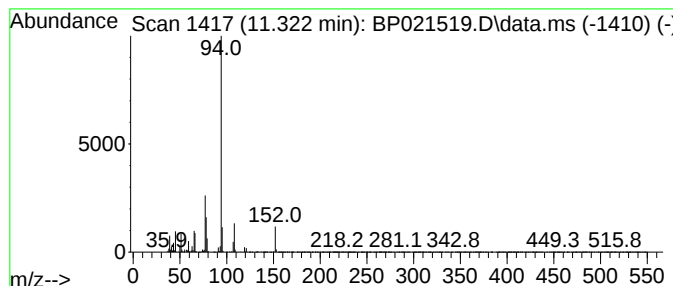
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.322	4.60 ng	814265	Naphthalene-d8	10.587

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	95
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	58
5			Benzene, propoxy-	136	C9H12O	000622-85-5	53



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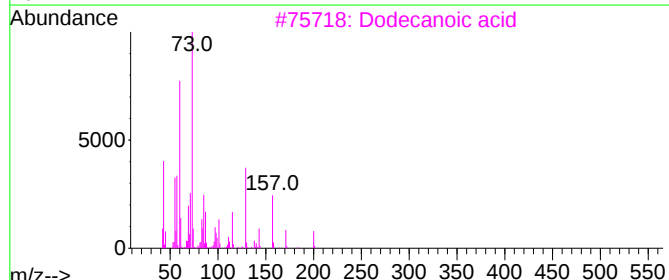
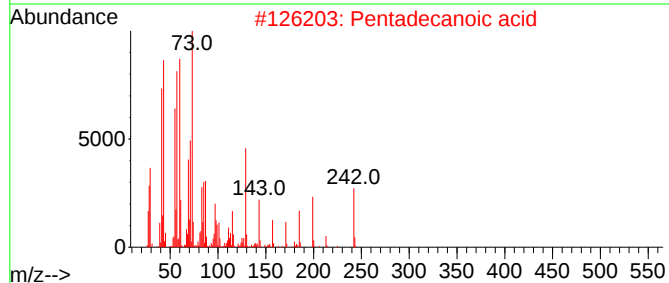
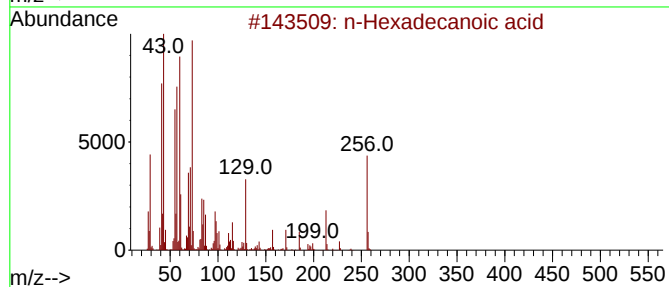
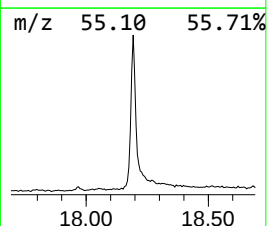
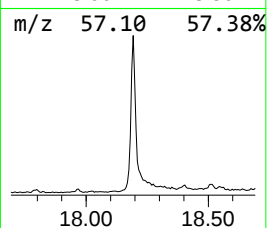
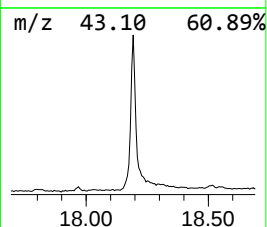
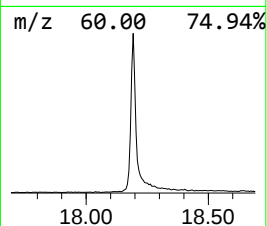
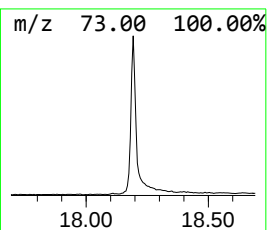
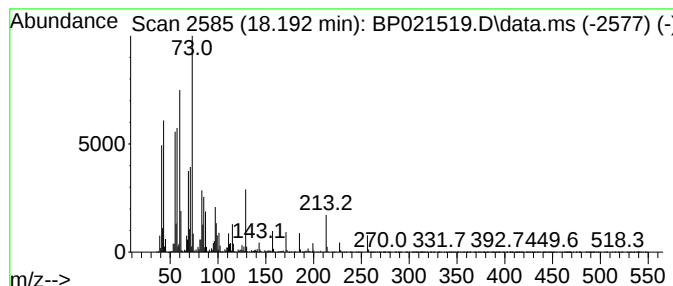
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.192	12.37 ng	3143700	Phenanthrene-d10	17.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3			Dodecanoic acid	200	C12H24O2	000143-07-7	53
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5			Tridecanoic acid	214	C13H26O2	000638-53-9	53



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ClientSampleId :
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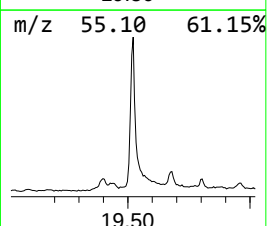
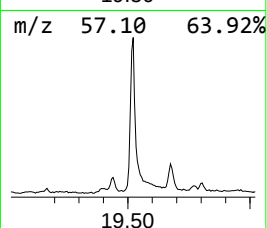
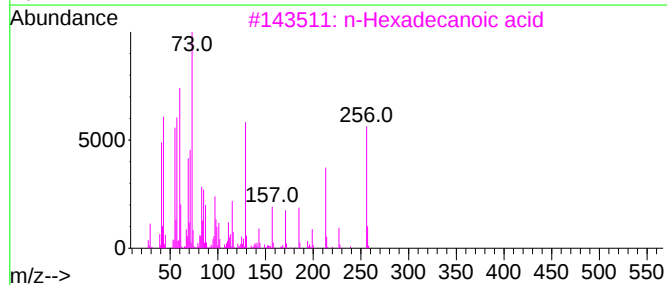
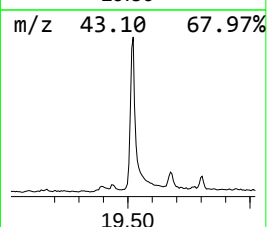
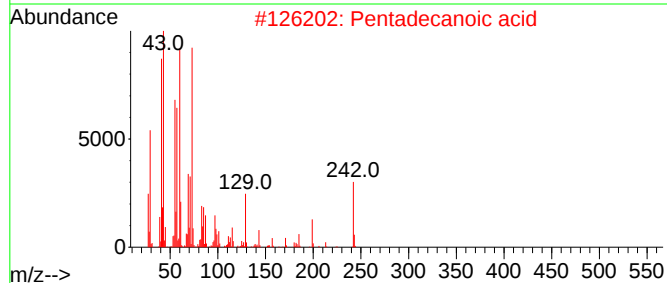
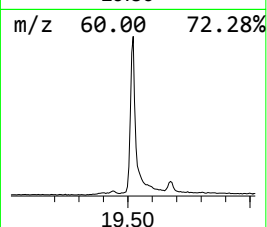
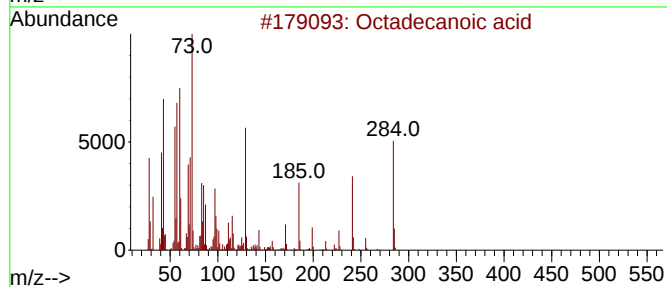
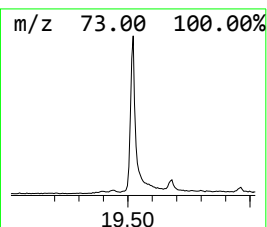
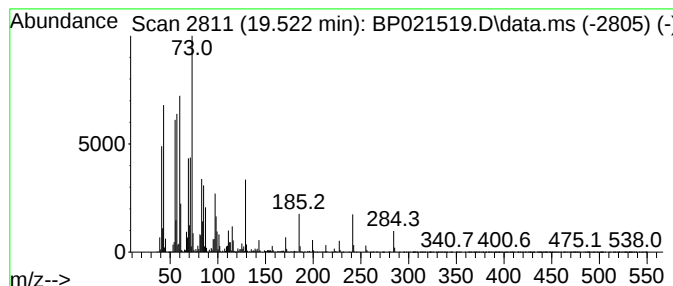
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.522	15.20 ng	3971770	Chrysene-d12	21.686

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	80
3			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
4			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
Data File : BP021519.D
Acq On : 15 Aug 2024 18:37
Operator : RC/JU
Sample : P3582-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-855-J-SO-1.5-2-081224

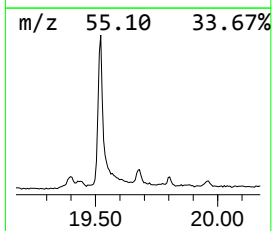
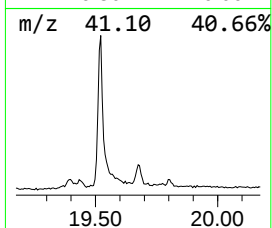
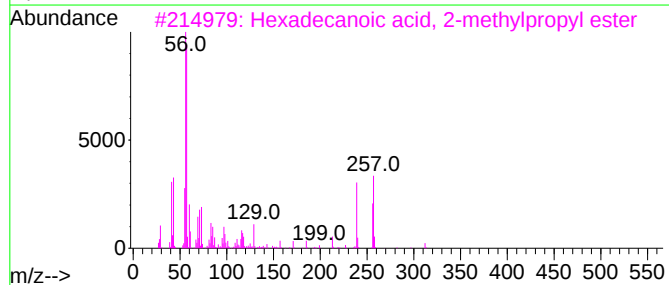
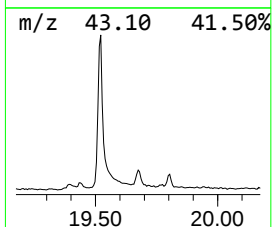
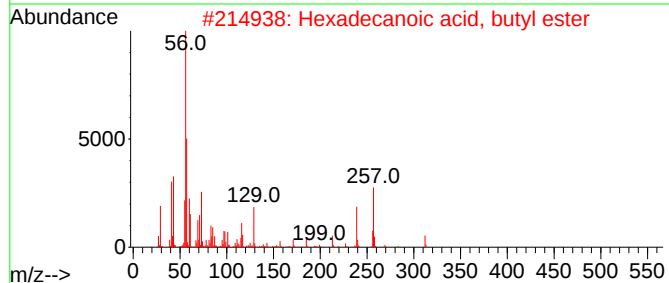
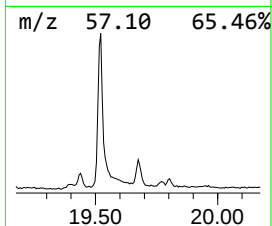
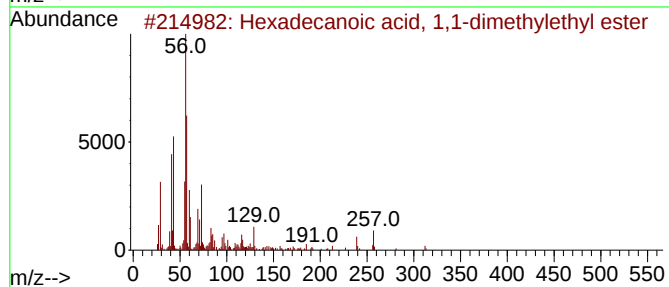
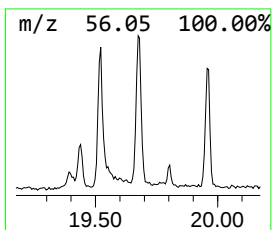
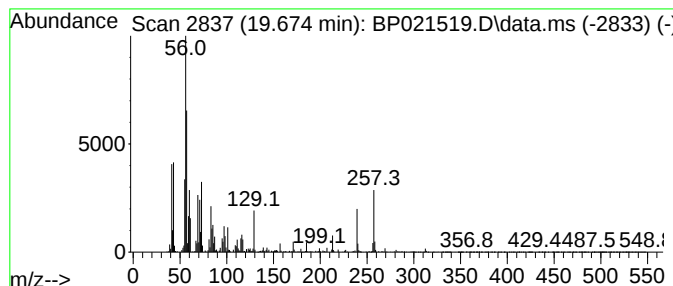
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, 1,1-dime... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.674	2.07 ng	541964	Chrysene-d12	21.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	96
2			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	90
4			1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	35
5			1-Decene, 9-methyl-	154	C11H22	061142-78-7	30



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
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Acq On : 15 Aug 2024 18:37
Operator : RC/JU
Sample : P3582-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

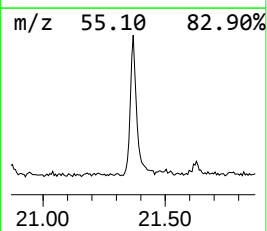
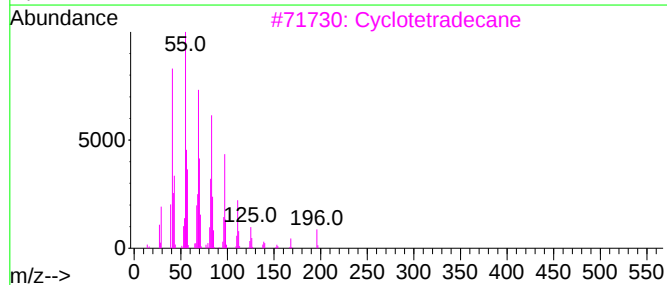
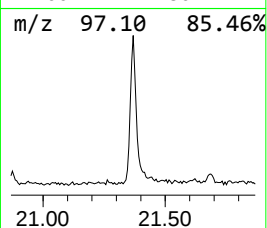
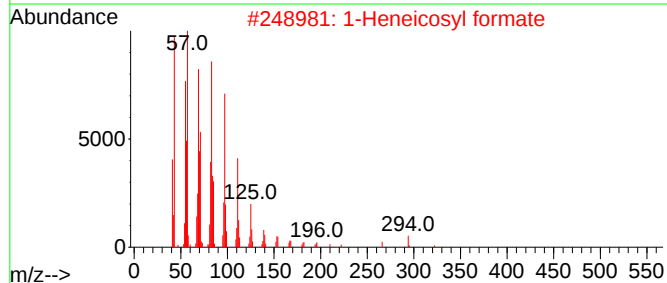
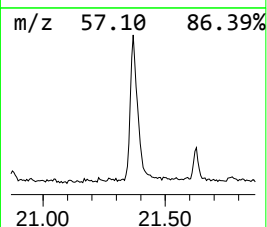
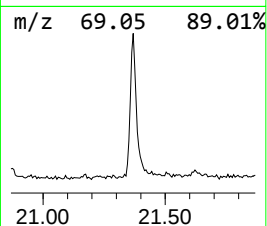
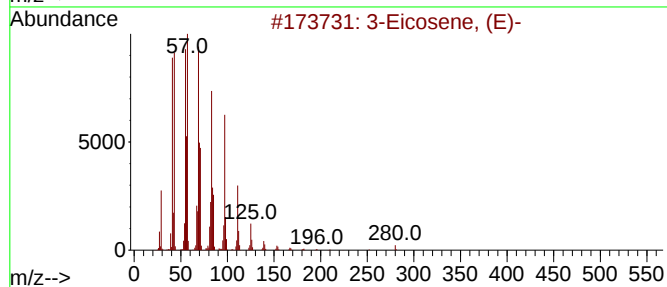
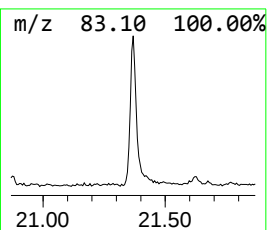
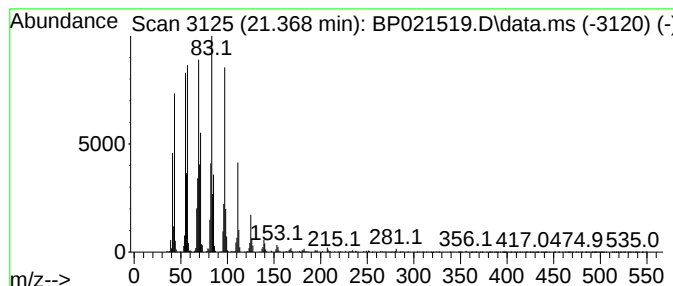
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ClientSampleId :
S-855-J-SO-1.5-2-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 3-Eicosene, (E)- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.369	5.31 ng	1386890	Chrysene-d12		21.686	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-		280	C20H40	074685-33-9	99
2	1-Heneicosyl formate		340	C22H44O2	077899-03-7	94
3	Cyclotetradecane		196	C14H28	000295-17-0	93
4	Behenic alcohol		326	C22H46O	000661-19-8	91
5	n-Tetracosanol-1		354	C24H50O	000506-51-4	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
Data File : BP021519.D
Acq On : 15 Aug 2024 18:37
Operator : RC/JU
Sample : P3582-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-855-J-SO-1.5-2-081224

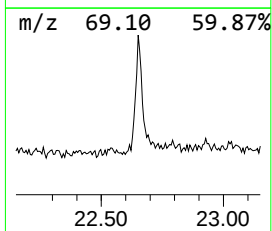
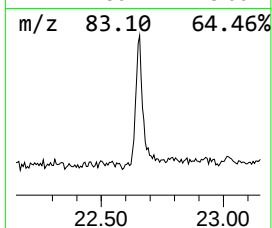
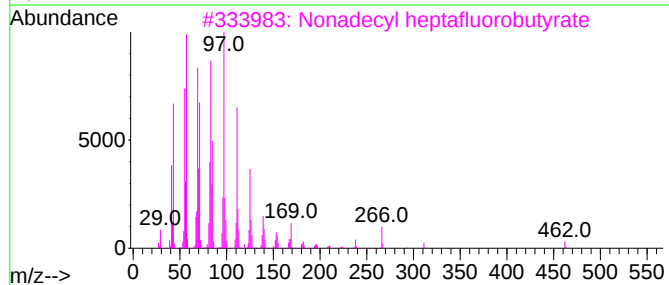
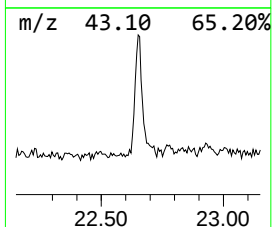
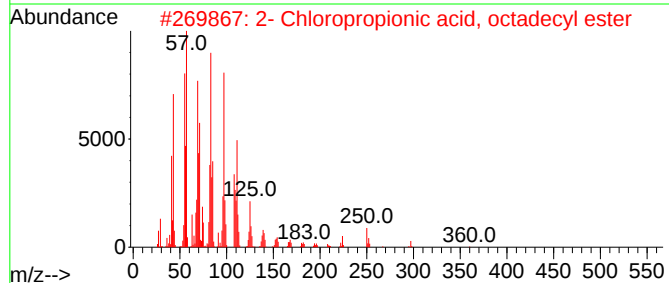
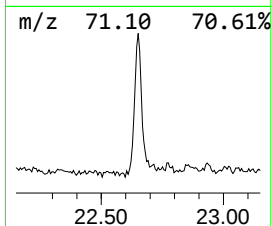
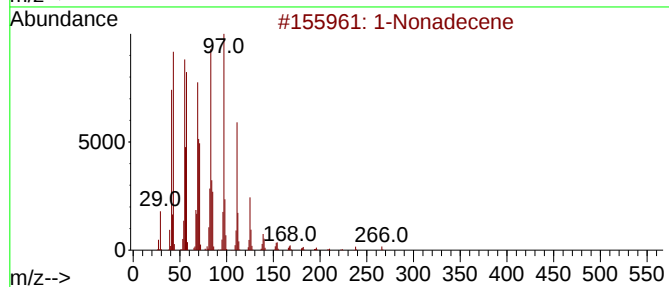
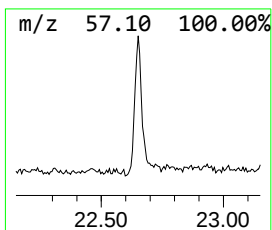
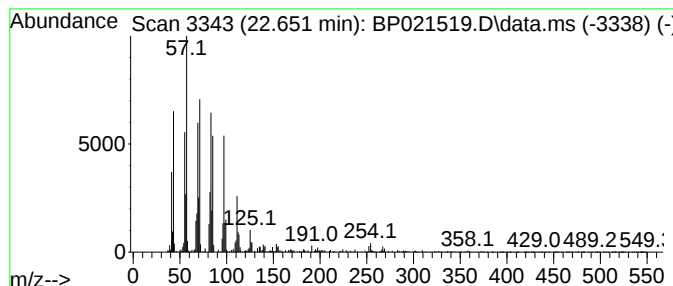
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1-Nonadecene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.651	2.16 ng	564893	Chrysene-d12	21.686

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Nonadecene			266	C19H38	018435-45-5	95
2	2- Chloropropionic acid, octadec...			360	C21H41ClO2	088104-31-8	89
3	Nonadecyl heptafluorobutyrate			480	C23H39F7O2	1000351-83-9	87
4	Nonadecyl trifluoroacetate			380	C21H39F3O2	1000351-76-3	87
5	E-15-Heptadecenal			252	C17H32O	1000130-97-9	86



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
Data File : BP021519.D
Acq On : 15 Aug 2024 18:37
Operator : RC/JU
Sample : P3582-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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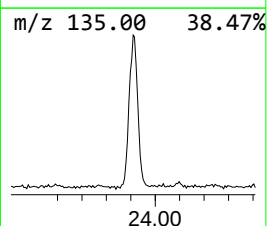
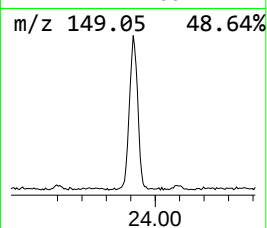
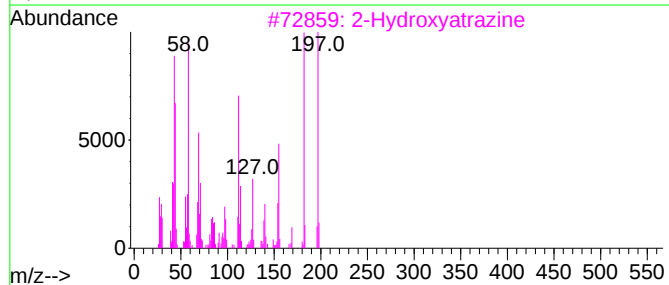
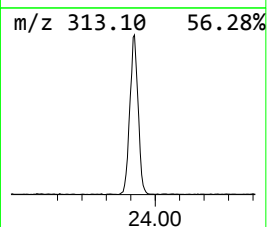
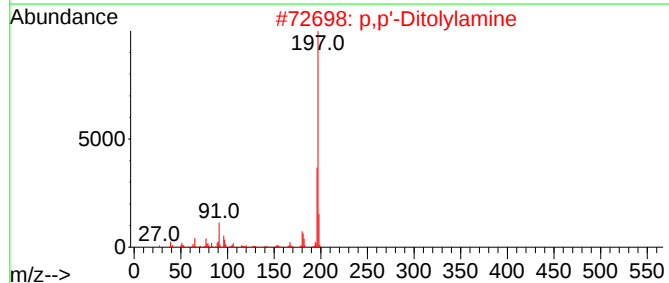
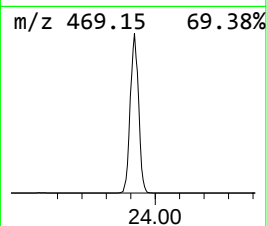
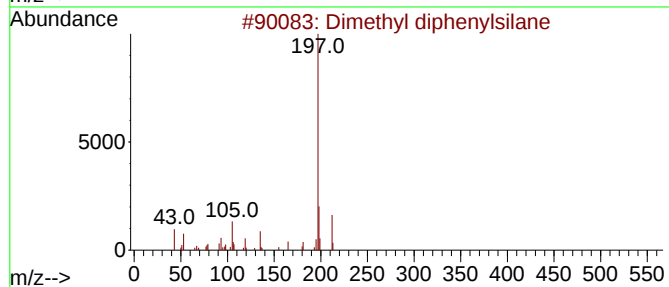
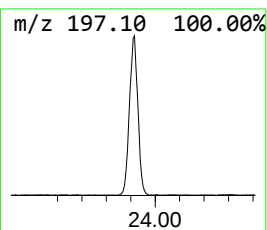
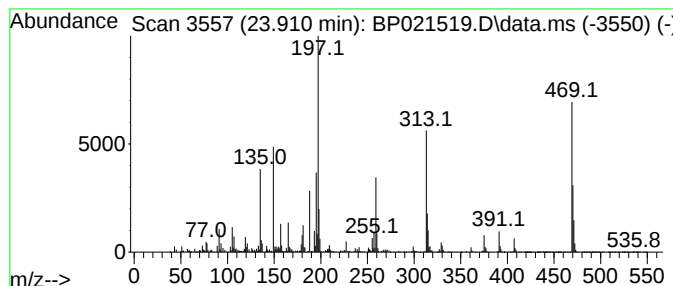
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown23.910 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.910	8.50 ng	2242330	Perylene-d12	25.080

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dimethyl diphenylsilane	212	C14H16Si	000778-24-5	22
2		p,p'-Ditolylamine	197	C14H15N	000620-93-9	18
3		2-Hydroxyatrazine	197	C8H15N5O	002163-68-0	15
4		4-Methyl-N-(4-methyl-2-pyridinyl...	262	C13H14N2O2S	331435-99-5	14
5		2,3-Dimethyl-1-(methyldiphenylsi...	280	C19H24Si	1000434-06-6	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP081524\
Data File : BP021519.D
Acq On : 15 Aug 2024 18:37
Operator : RC/JU
Sample : P3582-02
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-855-J-SO-1.5-2-081224

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP081324.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
Butane, 2-metho...	3.028	44.4	ng	5839190	1	7.799	2633280	20.0
Propylene Glycol	3.540	4.3	ng	571740	1	7.799	2633280	20.0
2-Pentanone, 4-...	4.934	3.2	ng	419386	1	7.799	2633280	20.0
1-Phenoxypropan...	11.322	4.6	ng	814265	2	10.587	3540860	20.0
n-Hexadecanoic ...	18.192	12.4	ng	3143700	4	17.245	5081110	20.0
Octadecanoic acid	19.522	15.2	ng	3971770	5	21.686	5225380	20.0
Hexadecanoic ac...	19.674	2.1	ng	541964	5	21.686	5225380	20.0
3-Eicosene, (E)-	21.369	5.3	ng	1386890	5	21.686	5225380	20.0
1-Nonadecene	22.651	2.2	ng	564893	5	21.686	5225380	20.0
unknown23.910	23.910	8.5	ng	2242330	6	25.080	5277290	20.0