

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
 Data File : BP003983.D
 Acq On : 17 Nov 2020 19:36
 Operator : CG/JU
 Sample : L4768-01
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 TR-05-111620

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\8270-BP110320.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003983.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.928	3	7	22	rVB	5343784	7010754	100.00%	14.467%
2	3.087	27	34	44	rVB	104049	217543	3.10%	0.449%
3	3.175	44	49	56	rBV	379153	503565	7.18%	1.039%
4	3.769	145	150	159	rBV	45714	70189	1.00%	0.145%
5	5.805	489	496	508	rBV	2381773	3564847	50.85%	7.356%
6	7.452	768	776	790	rBV	2219324	3741507	53.37%	7.721%
7	7.852	839	844	851	rBV	107813	161551	2.30%	0.333%
8	8.281	909	917	924	rBV	560783	883995	12.61%	1.824%
9	9.446	1100	1115	1125	rBV	1447596	2412122	34.41%	4.977%
10	11.110	1390	1398	1405	rBV	702861	1235284	17.62%	2.549%
11	13.528	1801	1809	1828	rBV	3159796	4661306	66.49%	9.619%
12	14.328	1940	1945	1952	rBV	619018	822777	11.74%	1.698%
13	14.904	2037	2043	2049	rBV	1032665	1512926	21.58%	3.122%
14	14.969	2049	2054	2061	rVB	81446	118477	1.69%	0.244%
15	15.298	2104	2110	2116	rVB	49611	75942	1.08%	0.157%
16	15.945	2215	2220	2227	rBV	58514	93166	1.33%	0.192%
17	16.386	2289	2295	2309	rBV	2202733	3287338	46.89%	6.783%
18	17.639	2502	2508	2512	rBV	1211090	1702982	24.29%	3.514%
19	17.680	2512	2515	2519	rVB	180948	239821	3.42%	0.495%
20	17.769	2527	2530	2536	rVB	58189	80669	1.15%	0.166%
21	18.257	2609	2613	2619	rBV	388337	443517	6.33%	0.915%
22	18.486	2648	2652	2656	rBV	52368	80117	1.14%	0.165%
23	18.533	2657	2660	2665	rVB2	54424	72394	1.03%	0.149%
24	18.674	2679	2684	2688	rBV4	65746	137757	1.96%	0.284%
25	19.227	2775	2778	2783	rBV	265212	325180	4.64%	0.671%
26	19.339	2789	2797	2800	rBV	2015402	2476493	35.32%	5.110%
27	19.369	2800	2802	2814	rVB2	1204649	1439058	20.53%	2.970%
28	19.492	2819	2823	2828	rBV2	218471	257868	3.68%	0.532%
29	19.616	2839	2844	2848	rBV	372283	485707	6.93%	1.002%
30	19.657	2848	2851	2855	rVB2	80443	94218	1.34%	0.194%
31	19.833	2878	2881	2885	rBV3	58849	72709	1.04%	0.150%
32	19.963	2899	2903	2910	rVB	350096	457173	6.52%	0.943%
33	20.139	2928	2933	2938	rVB	4557223	5452295	77.77%	11.251%
34	21.321	3131	3134	3144	rVB2	667996	883563	12.60%	1.823%
35	21.674	3188	3194	3198	rBV	1271133	1859813	26.53%	3.838%
36	24.162	3611	3617	3624	rVB	781590	1526374	21.77%	3.150%

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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\8270-BP110320.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

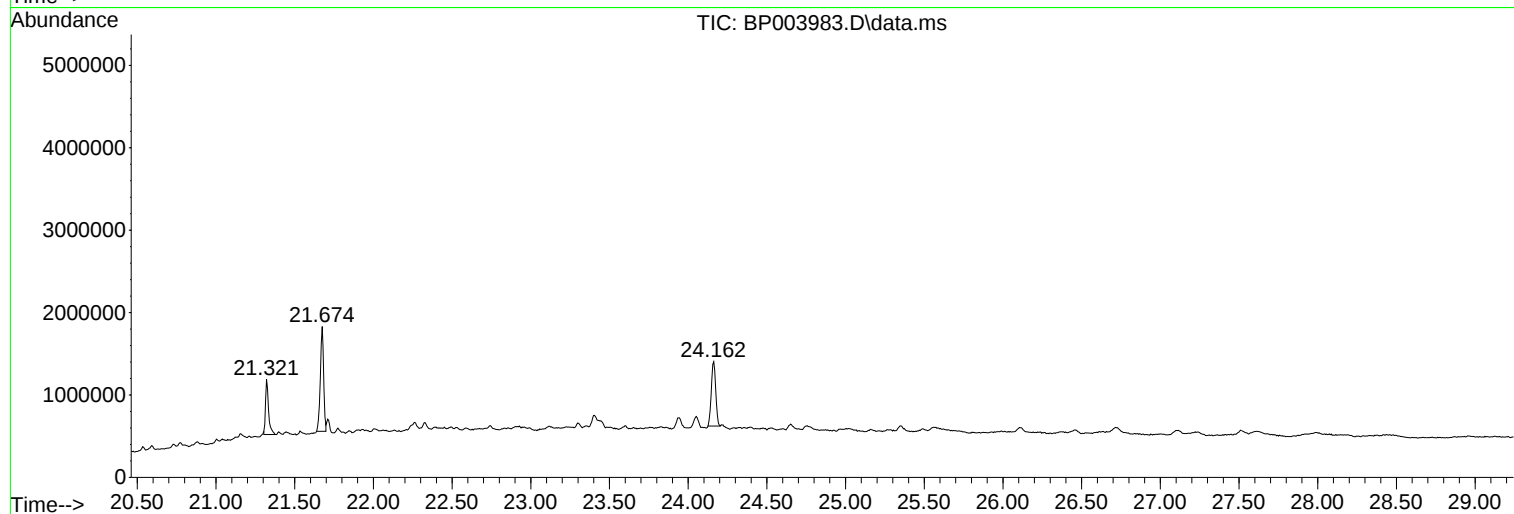
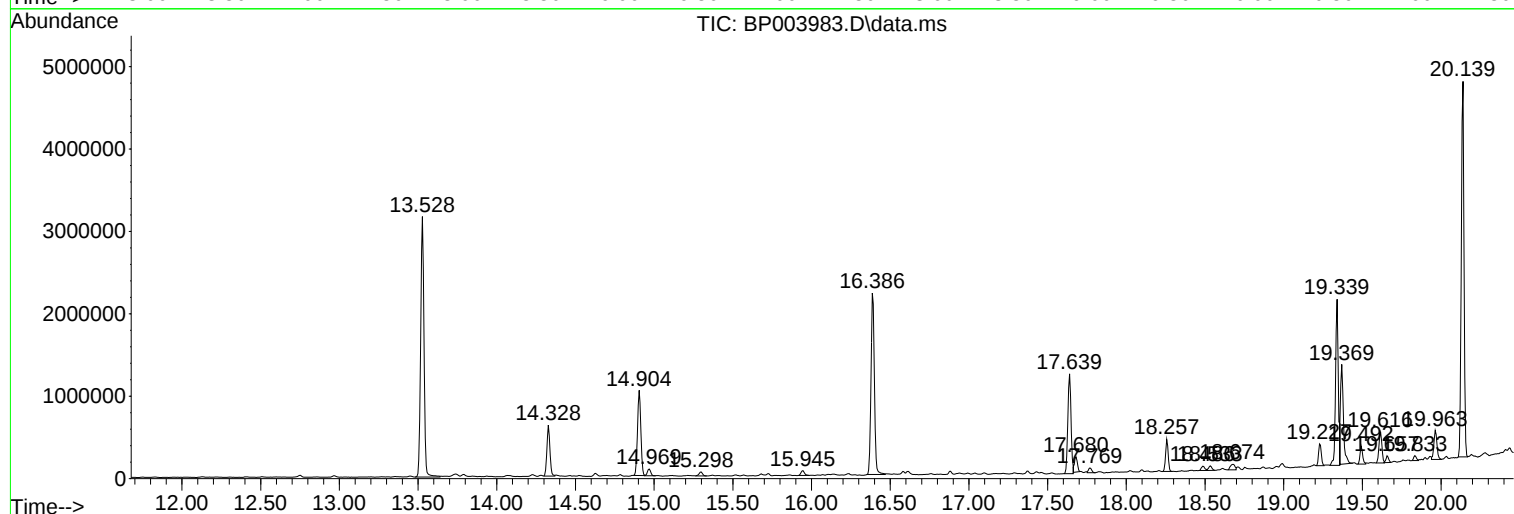
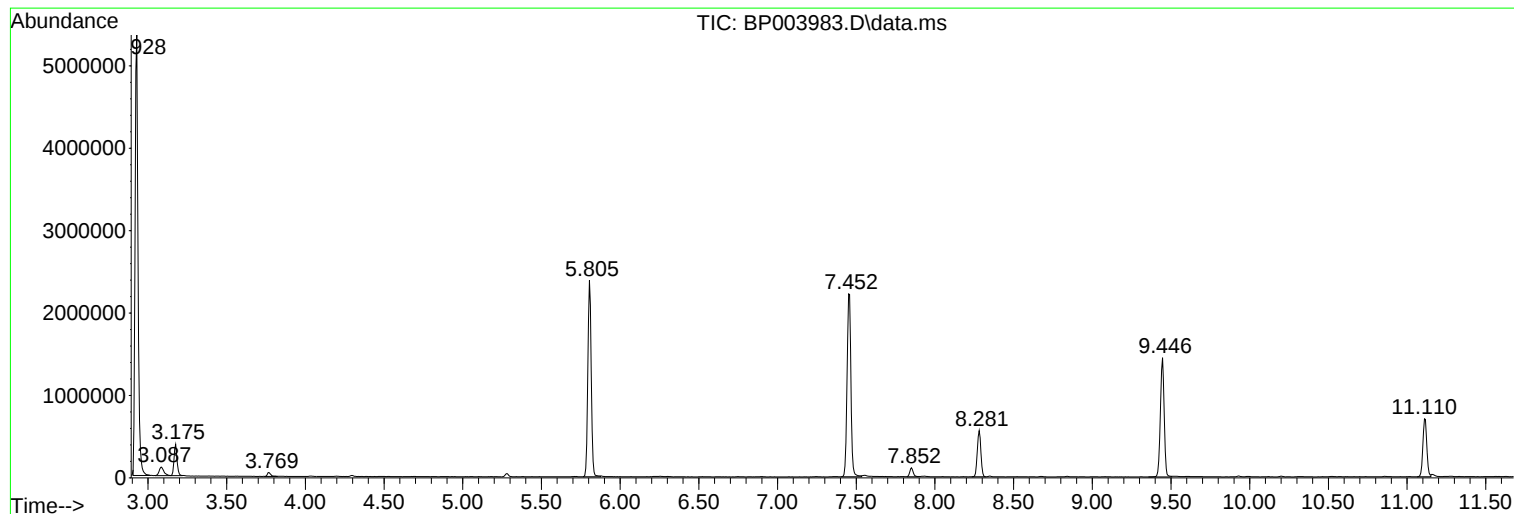
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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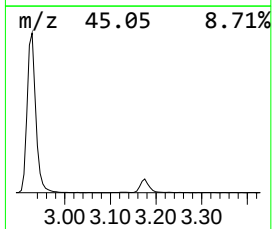
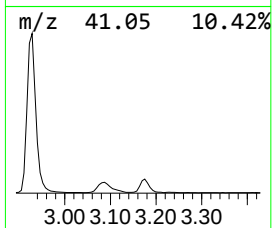
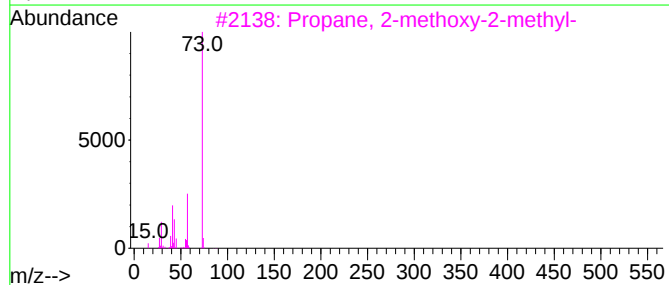
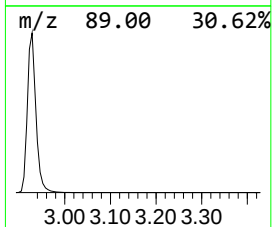
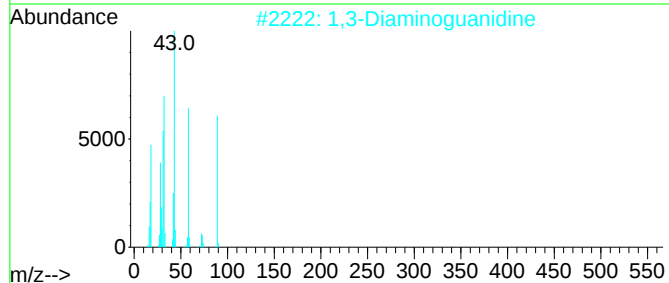
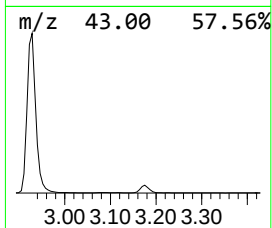
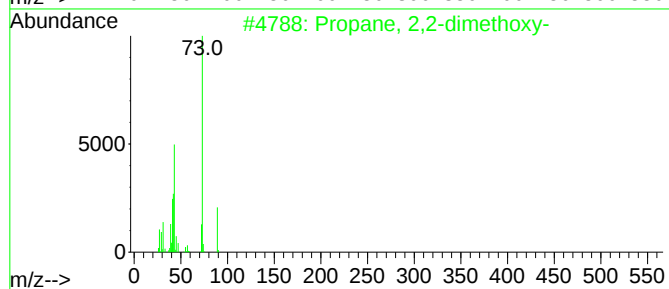
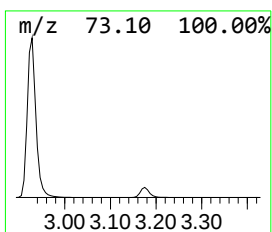
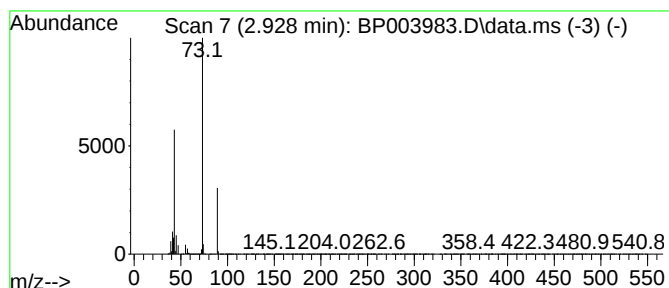
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.928	158.62 ng	7010750	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
3			Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5			1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrC13O2	1000115-31-4	9



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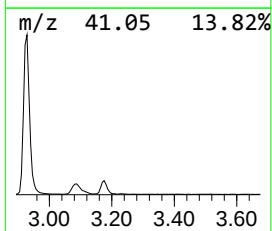
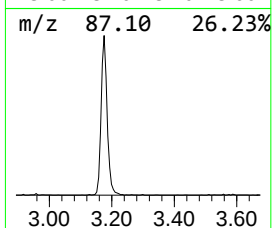
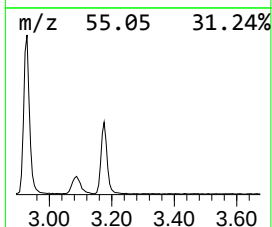
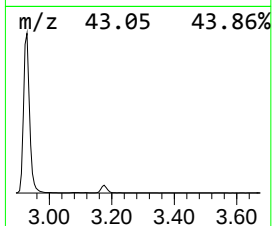
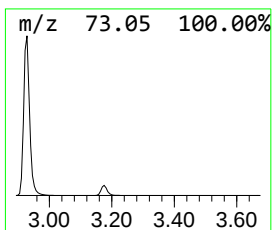
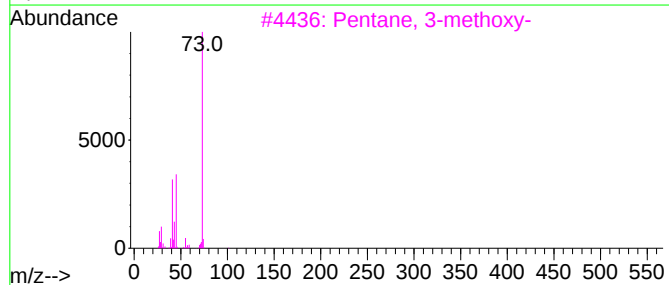
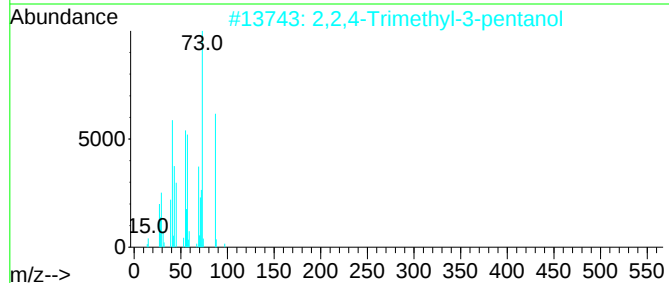
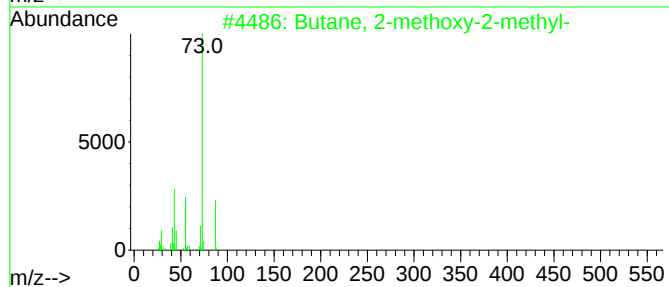
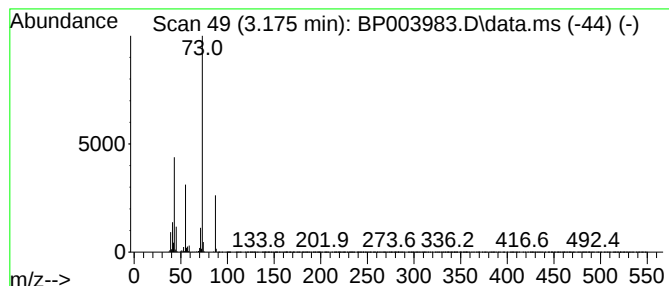
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.175	11.39 ng	503565	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
4			N-Ethylformamide	73	C3H7NO	000627-45-2	9
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9



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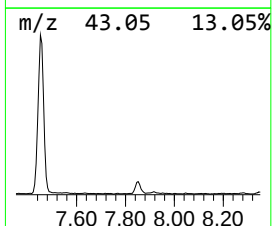
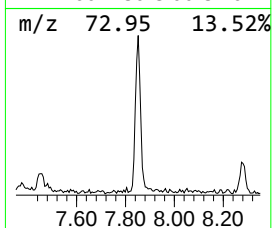
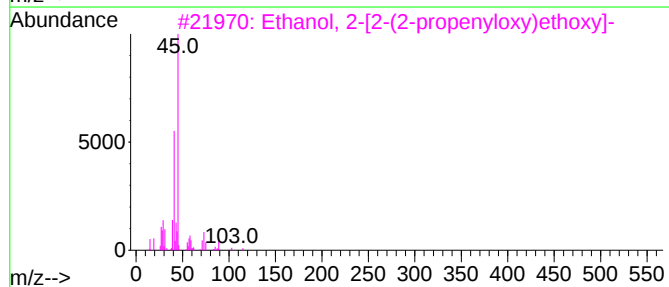
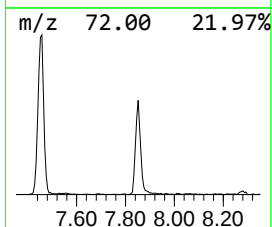
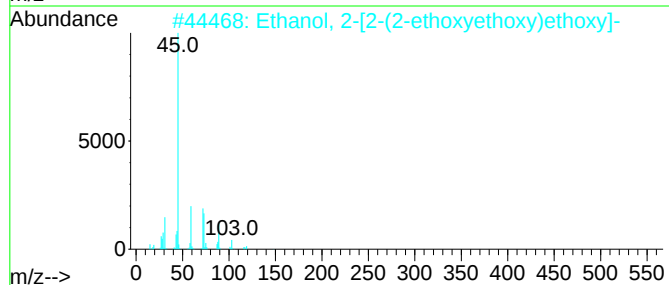
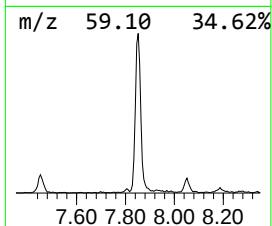
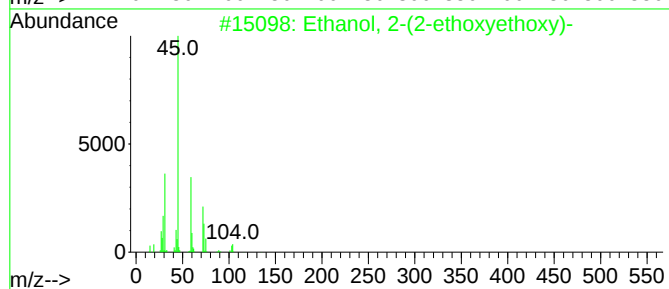
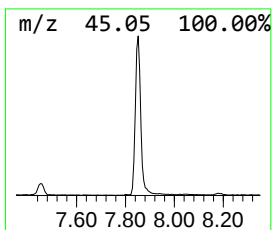
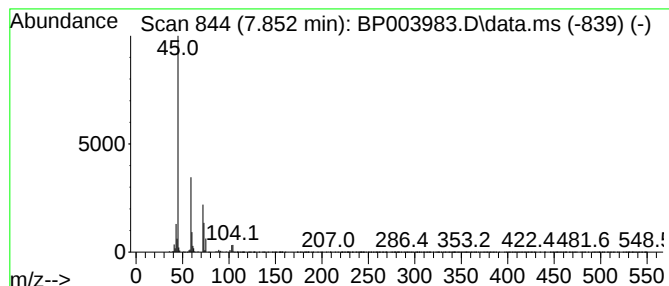
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.852	3.66 ng	161551	1,4-Dichlorobenzene-d4	8.281

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45
3			Ethanol, 2-[2-(2-propenyloxy)eth...	146	C7H14O3	015075-50-0	40
4			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	38
5			Ethyl ether	74	C4H10O	000060-29-7	33



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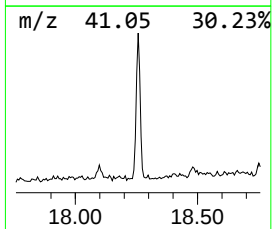
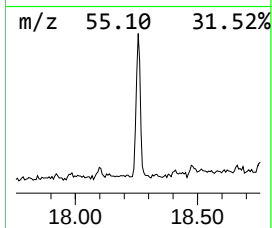
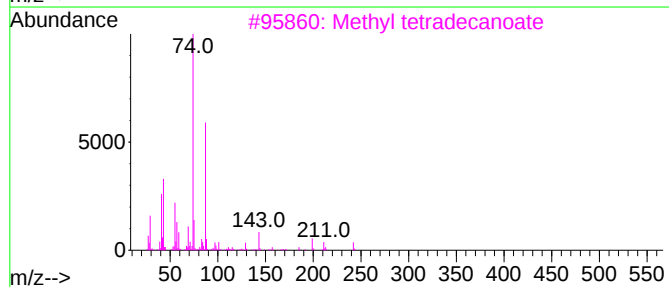
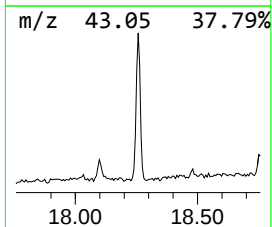
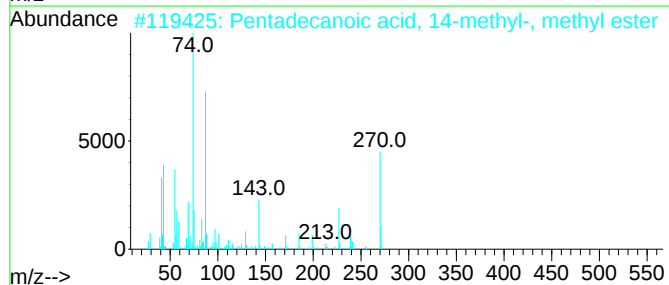
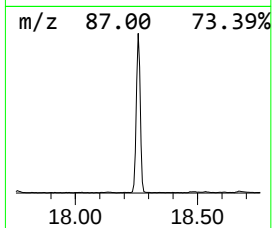
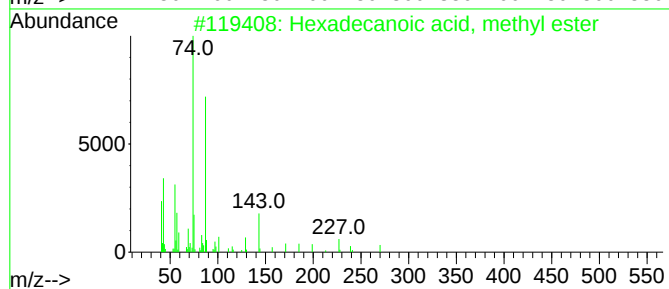
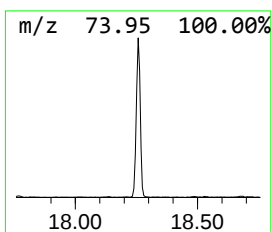
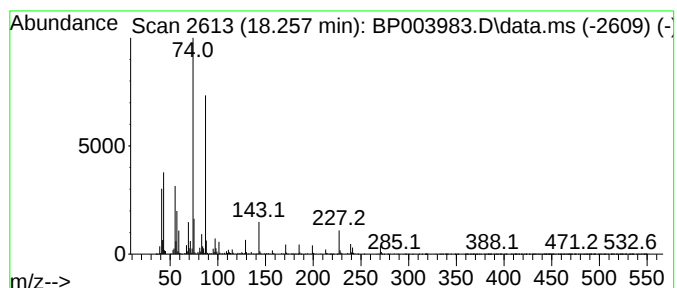
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Hexadecanoic acid, methyl e... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.257	5.21 ng	443517	Phenanthrene-d10	17.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	94
3			Methyl tetradecanoate	242	C15H30O2	000124-10-7	87
4			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	86
5			Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	80



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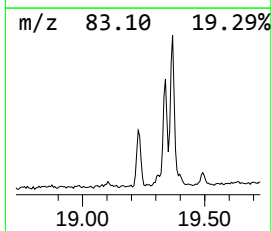
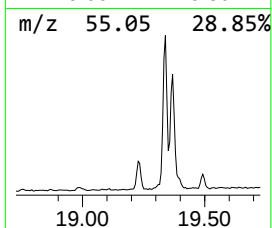
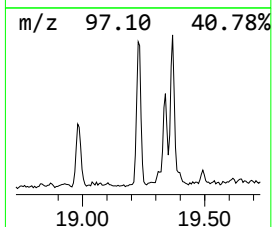
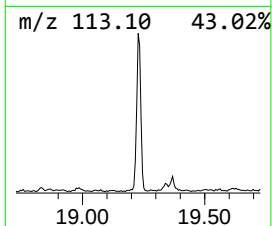
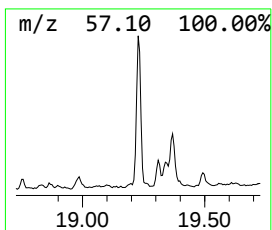
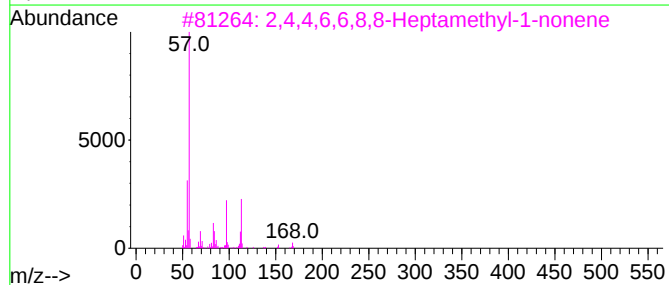
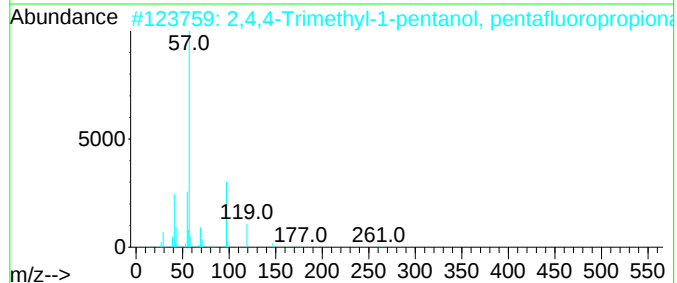
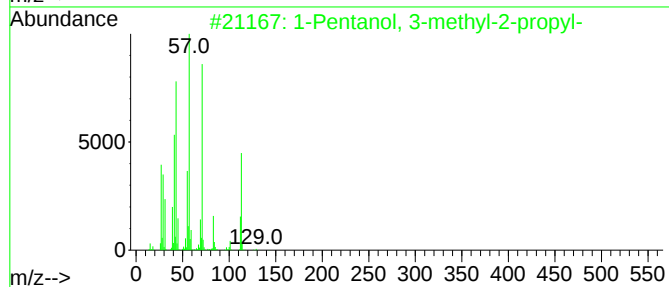
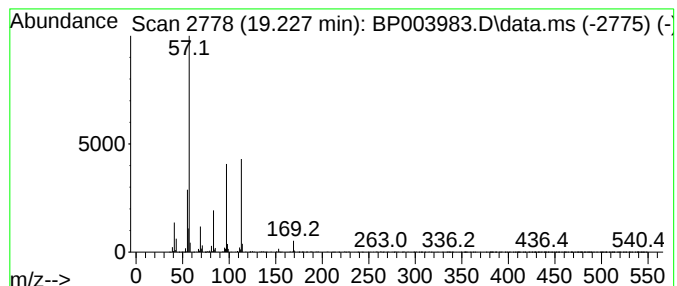
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown19.227 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.227	3.82 ng	325180	Phenanthrene-d10	17.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentanol, 3-methyl-2-propyl-	144	C9H20O	054004-40-9	40		
2	2,4,4-Trimethyl-1-pentanol, pent...	276	C11H17F5O2	1000365-51-0	38		
3	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	38		
4	2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	27		
5	Formic acid, 2,4,4-trimethylpent...	158	C9H18O2	1000368-95-2	25		



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
Data File : BP003983.D
Acq On : 17 Nov 2020 19:36
Operator : CG/JU
Sample : L4768-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

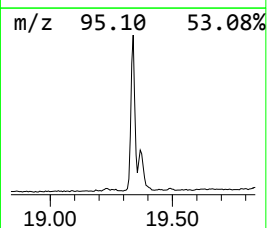
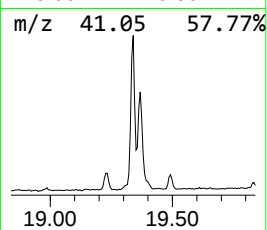
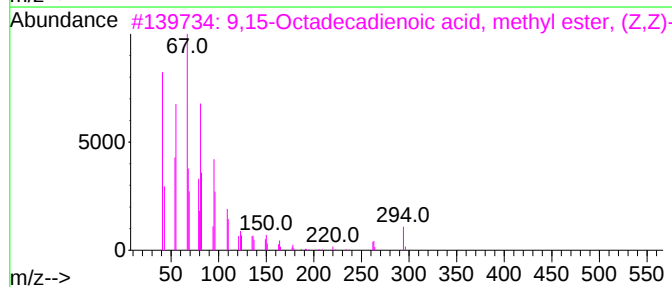
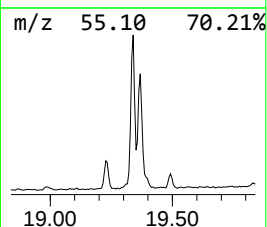
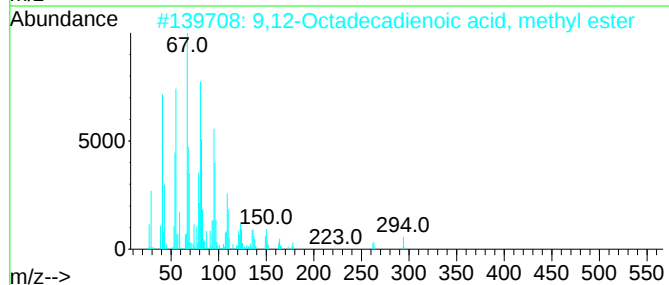
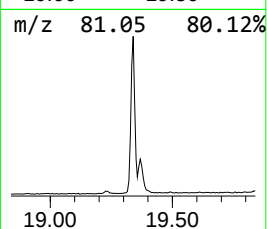
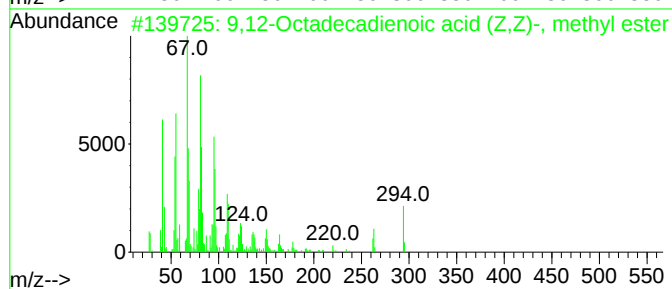
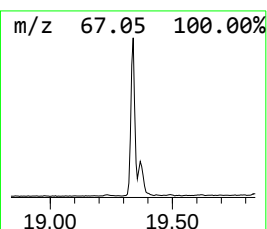
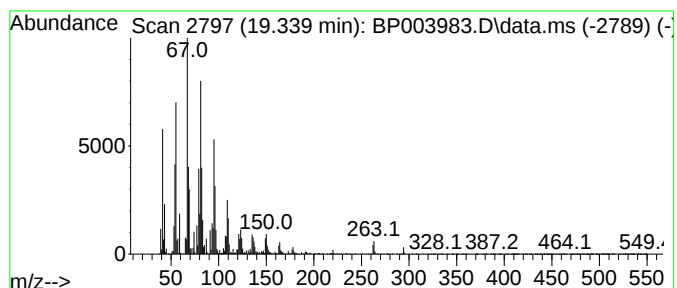
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ClientSampleId :
TR-05-111620

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9,12-Octadecadienoic acid (... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.339	29.08 ng	2476490	Phenanthrene-d10	17.639	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9,12-Octadecadienoic acid (Z,Z)-...	294	C19H34O2	000112-63-0	99
2	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002462-85-3	99
3	9,15-Octadecadienoic acid, methy...	294	C19H34O2	017309-05-6	99
4	9,12-Octadecadienoic acid, methy...	294	C19H34O2	002566-97-4	99
5	Methyl 9-cis,11-trans-octadecadi...	294	C19H34O2	1000336-44-0	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
Data File : BP003983.D
Acq On : 17 Nov 2020 19:36
Operator : CG/JU
Sample : L4768-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-111620

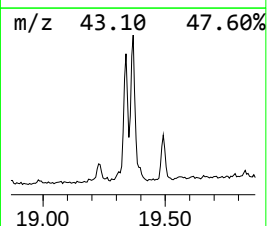
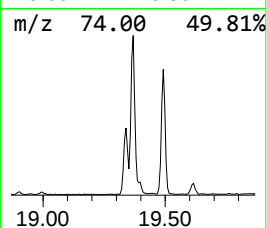
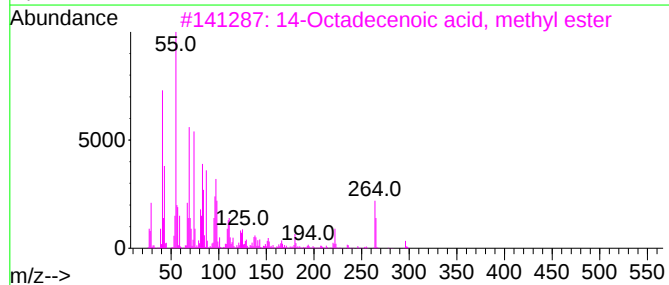
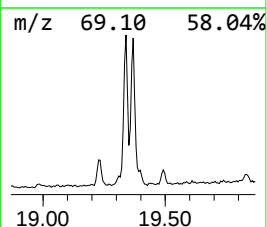
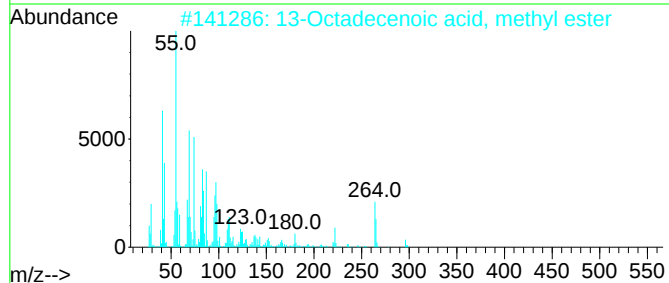
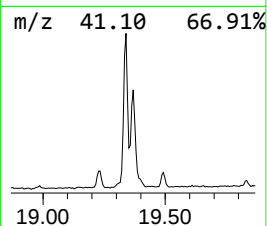
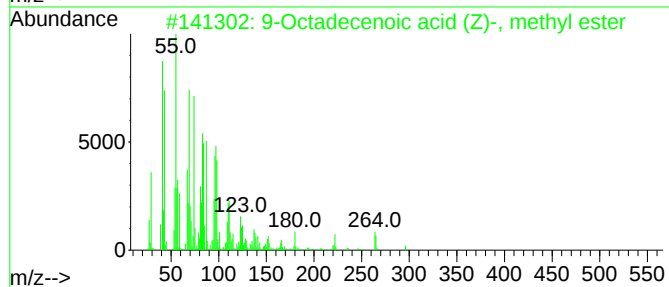
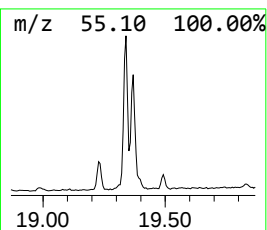
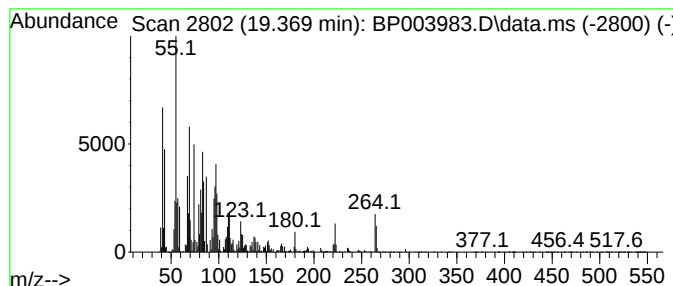
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenoic acid (Z)-, m... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.369	16.90 ng	1439060	Phenanthrene-d10	17.639

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2		13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	99
3		14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	98
4		16-Octadecenoic acid, methyl ester	296	C19H36O2	056554-49-5	98
5		6-Octadecenoic acid, methyl este...	296	C19H36O2	002777-58-4	98



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
Data File : BP003983.D
Acq On : 17 Nov 2020 19:36
Operator : CG/JU
Sample : L4768-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-111620

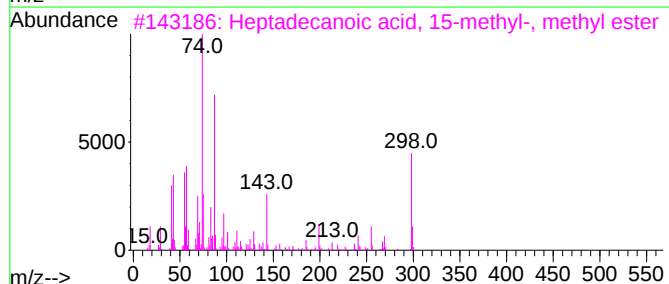
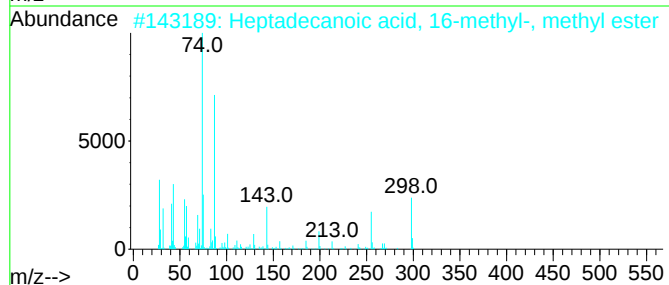
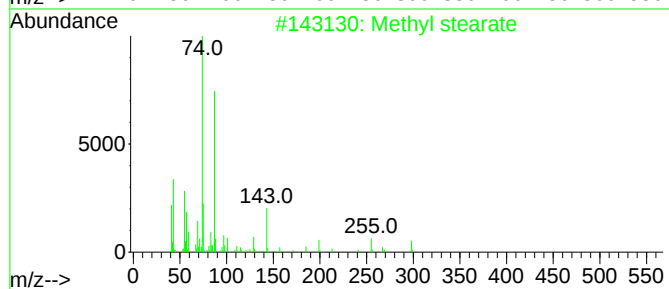
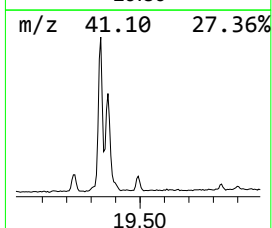
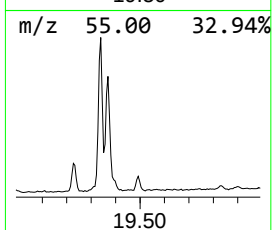
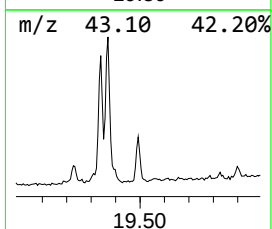
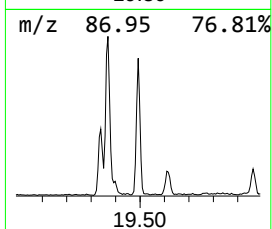
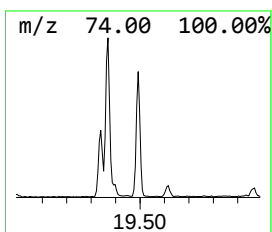
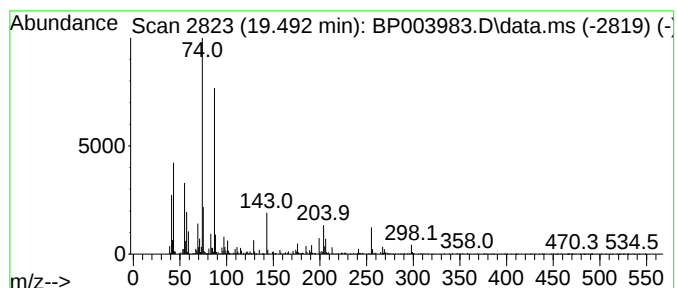
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Methyl stearate Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.492	3.03 ng	257868	Phenanthrene-d10	17.639

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl stearate	298	C19H38O2	000112-61-8	98
2			Heptadecanoic acid, 16-methyl-, ...	298	C19H38O2	005129-61-3	93
3			Heptadecanoic acid, 15-methyl-, ...	298	C19H38O2	054833-55-5	93
4			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	91
5			Heptadecanoic acid, methyl ester	284	C18H36O2	001731-92-6	81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
Data File : BP003983.D
Acq On : 17 Nov 2020 19:36
Operator : CG/JU
Sample : L4768-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-111620

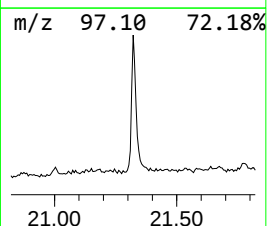
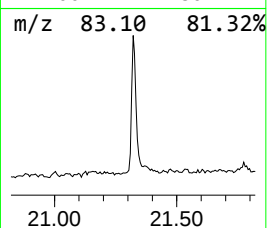
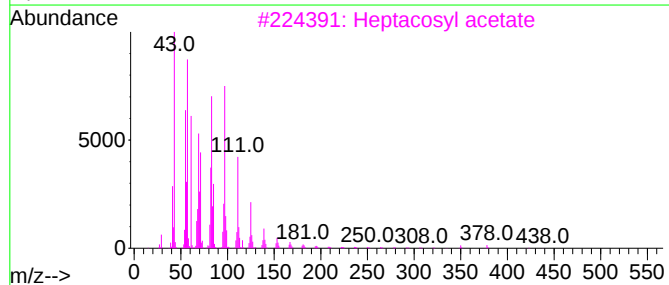
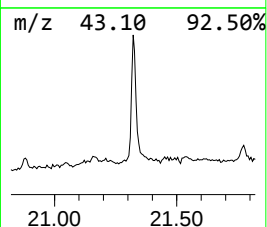
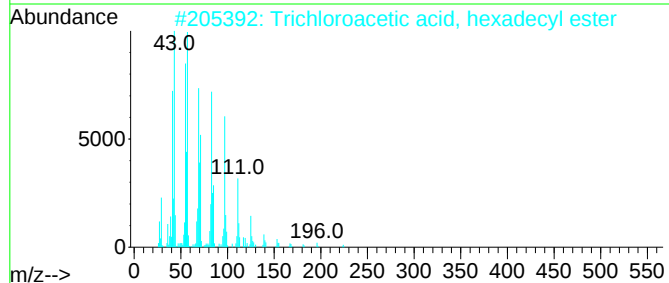
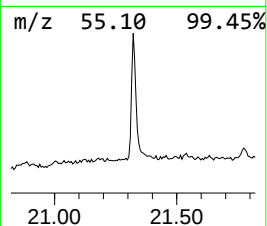
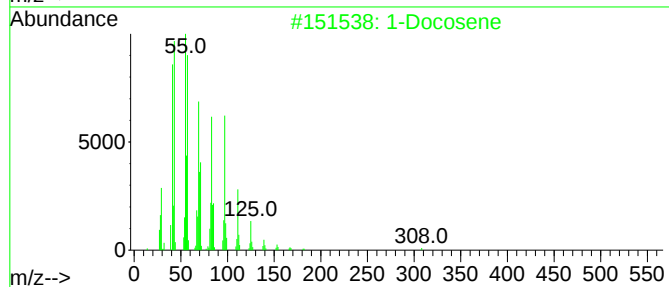
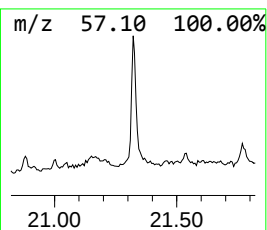
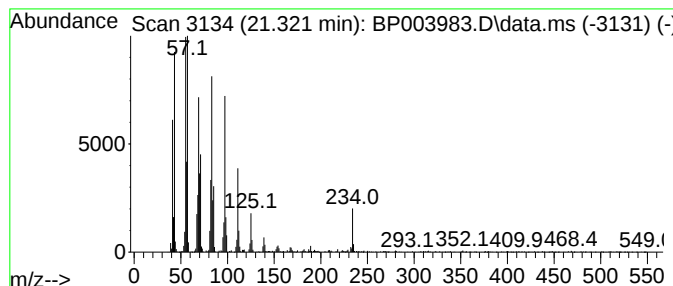
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1-Docosene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.321	9.50 ng	883563	Chrysene-d12	21.674

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Docosene	308	C22H44	001599-67-3	93
2		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	93
3		Heptacosyl acetate	438	C29H58O2	1000351-78-2	91
4		1-Triacontanol	438	C30H62O	000593-50-0	91
5		Octacosyl acetate	452	C30H60O2	018206-97-8	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP111720\
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Operator : CG/JU
Sample : L4768-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
TR-05-111620

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-di...	2.928	158.6	ng	7010750	1	8.281	883995	20.0
Butane, 2-metho...	3.175	11.4	ng	503565	1	8.281	883995	20.0
Ethanol, 2-(2-e...	7.852	3.7	ng	161551	1	8.281	883995	20.0
Hexadecanoic ac...	18.257	5.2	ng	443517	4	17.639	1702980	20.0
unknown19.227	19.227	3.8	ng	325180	4	17.639	1702980	20.0
9,12-Octadecadi...	19.339	29.1	ng	2476490	4	17.639	1702980	20.0
9-Octadecenoic ...	19.369	16.9	ng	1439060	4	17.639	1702980	20.0
Methyl stearate	19.492	3.0	ng	257868	4	17.639	1702980	20.0
1-Docosene	21.321	9.5	ng	883563	5	21.674	1859810	20.0