

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
 Data File : BP013453.D
 Acq On : 11 Jan 2023 20:29
 Operator : CG/JU
 Sample : 01064-08
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-14-03

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-BP121322.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP013453.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.434	203	212	236	rBV	4410106	12963958	5.16%	1.386%
2	5.011	305	310	322	rVB	2374024	3900359	1.55%	0.417%
3	5.475	384	389	415	rVB	6242118	10311661	4.10%	1.102%
4	7.087	632	663	675	rBV2	9139313	26251408	10.44%	2.806%
5	7.922	797	805	812	rVB	1712044	2742525	1.09%	0.293%
6	8.540	892	910	926	rBV2	2136700	6653963	2.65%	0.711%
7	9.093	996	1004	1024	rVB2	4912644	11700799	4.65%	1.251%
8	9.246	1024	1030	1041	rBV	1464675	2805448	1.12%	0.300%
9	10.105	1162	1176	1180	rBV	1937830	5110940	2.03%	0.546%
10	10.734	1277	1283	1293	rVV	2598474	4445489	1.77%	0.475%
11	11.404	1391	1397	1406	rBV2	1916316	3746606	1.49%	0.400%
12	11.575	1412	1426	1432	rBV	2807297	7163350	2.85%	0.766%
13	12.369	1551	1561	1570	rBV	1503269	3027027	1.20%	0.324%
14	12.763	1622	1628	1634	rBV	2569866	4191333	1.67%	0.448%
15	12.863	1641	1645	1650	rVB	1766921	2645517	1.05%	0.283%
16	13.040	1663	1675	1689	rVB7	1240969	4226985	1.68%	0.452%
17	13.187	1694	1700	1707	rVB	11594478	16992467	6.76%	1.816%
18	14.181	1861	1869	1874	rBV2	3280193	6312678	2.51%	0.675%
19	14.569	1929	1935	1940	rBV	4450509	6542214	2.60%	0.699%
20	14.987	1998	2006	2013	rBV3	3082942	6116617	2.43%	0.654%
21	15.192	2036	2041	2045	rBV	2134427	2912899	1.16%	0.311%
22	16.063	2183	2189	2194	rBV	11922319	16989999	6.76%	1.816%
23	16.745	2295	2305	2317	rBV	21880759	45012075	17.91%	4.812%
24	17.328	2399	2404	2408	rBV	5930805	8409592	3.35%	0.899%
25	17.492	2424	2432	2443	rVB2	2237703	4055114	1.61%	0.433%
26	18.139	2529	2542	2548	rBV2	4660348	20078830	7.99%	2.146%
27	18.298	2549	2569	2575	rBV8	35008203	251362226	100.00%	26.869%
28	18.863	2661	2665	2670	rBV	4884936	6275723	2.50%	0.671%
29	19.222	2720	2726	2733	rVB	5312744	7263248	2.89%	0.776%
30	19.381	2736	2753	2756	rBV7	36241618	175160408	69.68%	18.724%
31	19.504	2764	2774	2787	rVB2	33249763	112666374	44.82%	12.043%
32	19.604	2787	2791	2802	rVB2	8298990	13073205	5.20%	1.397%
33	19.810	2822	2826	2833	rBV	10691503	12927744	5.14%	1.382%
34	19.886	2834	2839	2843	rVV	20199299	25798122	10.26%	2.758%
35	20.180	2885	2889	2894	rVB2	3855357	4839189	1.93%	0.517%
36	20.351	2916	2918	2922	rVB	3023023	3021605	1.20%	0.323%

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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\8270E-BP121322.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	20.416	2925	2929	2938	rVV	15537349	24274693	9.66%	2.595%
38	20.498	2939	2943	2952	rVV3	11162429	23865676	9.49%	2.551%
39	21.104	3043	3046	3050	rBV	3120772	3478703	1.38%	0.372%
40	21.222	3063	3066	3072	rVB	4119869	4784470	1.90%	0.511%
41	21.416	3094	3099	3104	rBV2	7885495	14604476	5.81%	1.561%
42	23.886	3515	3519	3525	rVB2	3598097	6796449	2.70%	0.727%

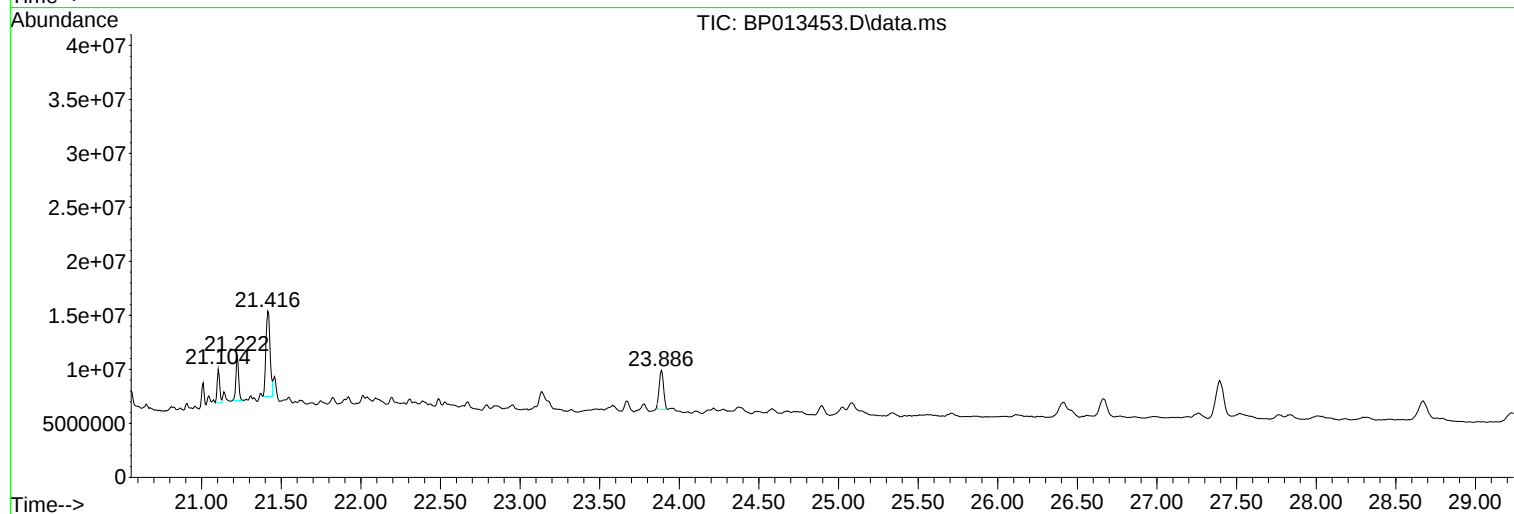
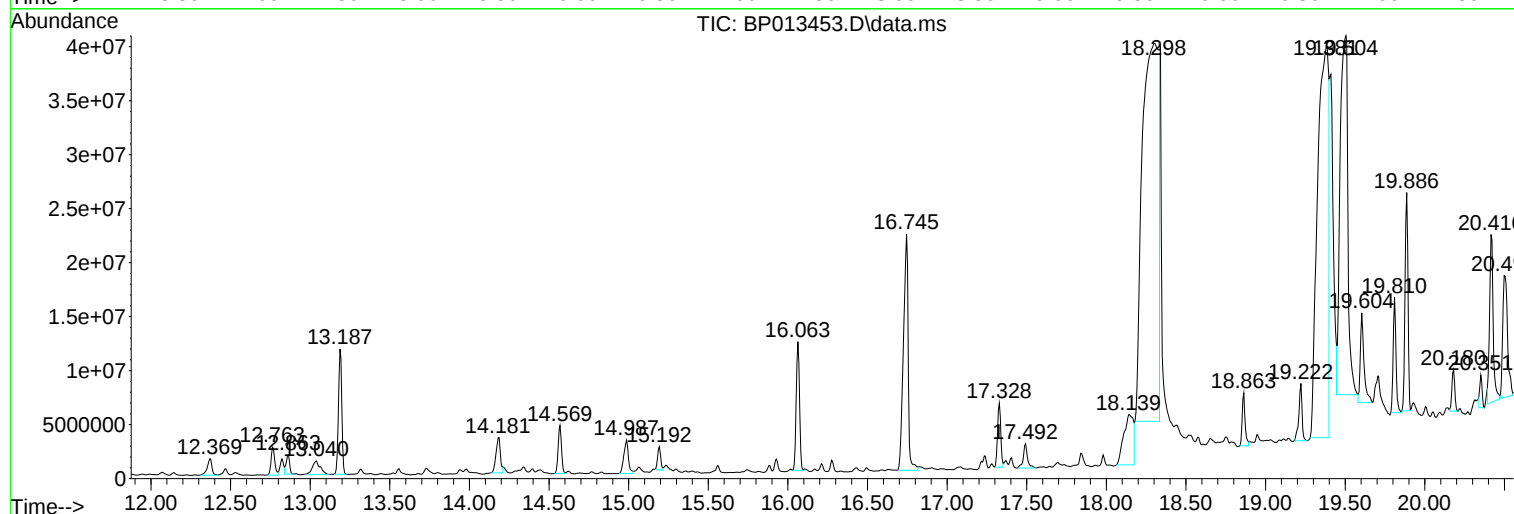
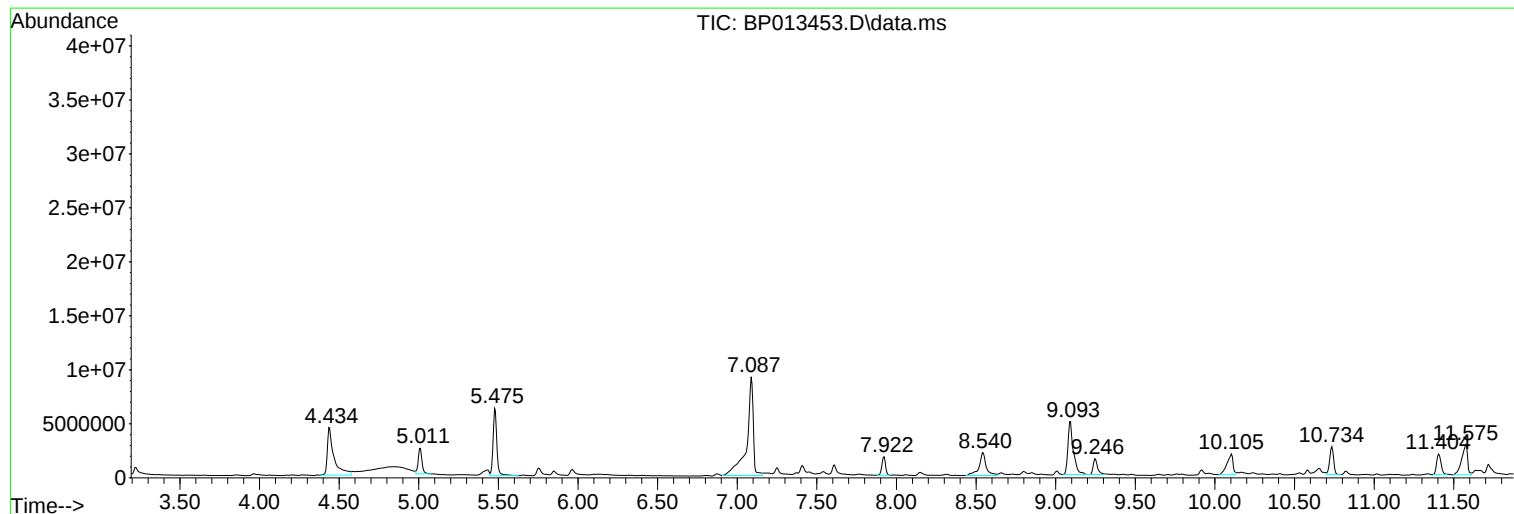
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Misc :
ALS Vial : 16 Sample Multiplier: 1

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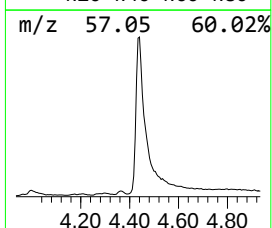
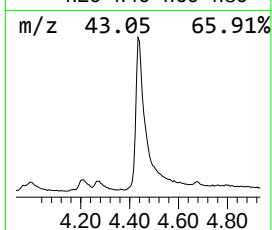
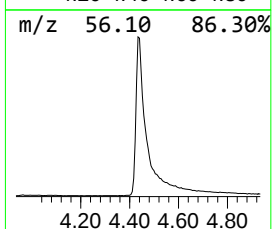
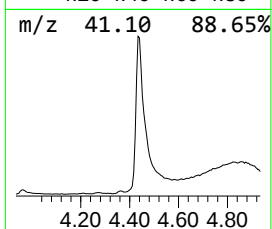
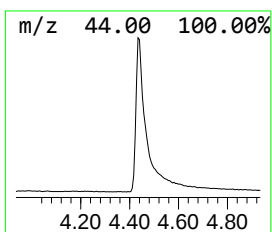
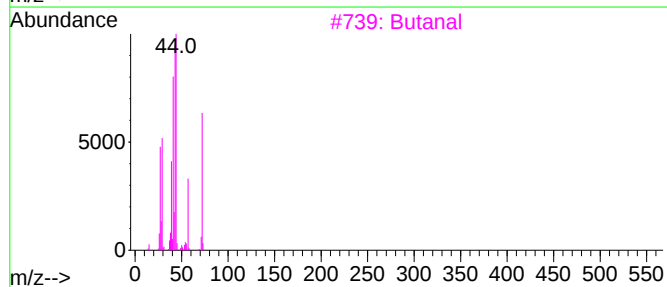
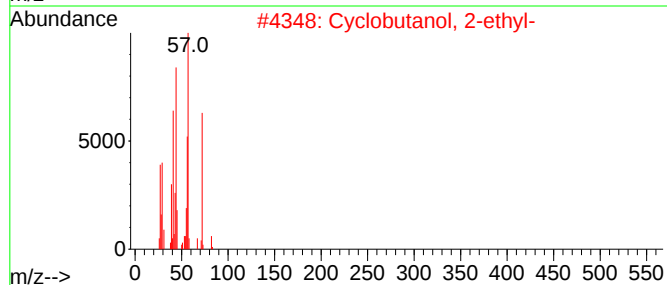
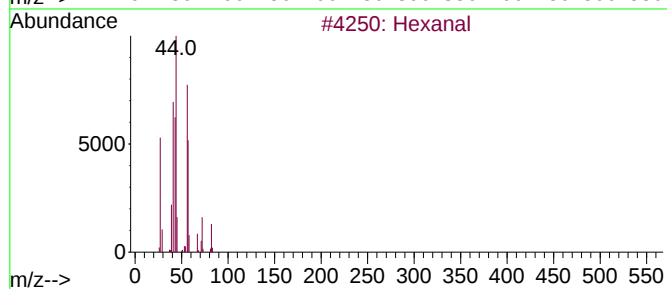
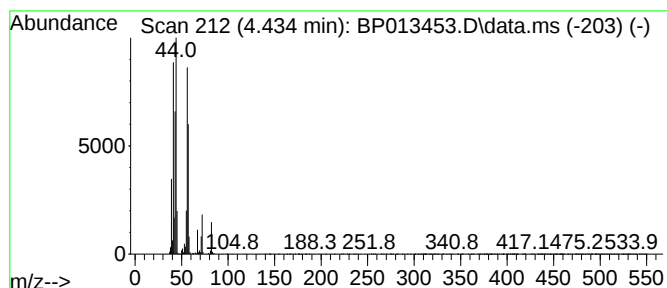
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.434	94.54 ng	12964000	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	90
2			Cyclobutanol, 2-ethyl-	100	C6H12O	035301-43-0	45
3			Butanal	72	C4H8O	000123-72-8	35
4			Cyanic acid, butyl ester	99	C5H9NO	001768-24-7	32
5			Cyclobutane	56	C4H8	000287-23-0	27



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Misc :
ALS Vial : 16 Sample Multiplier: 1

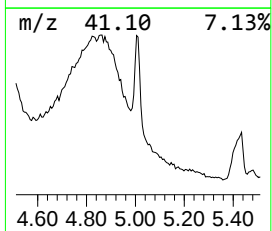
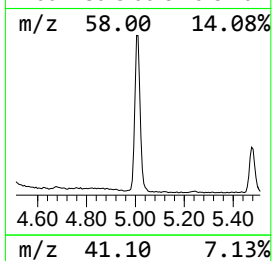
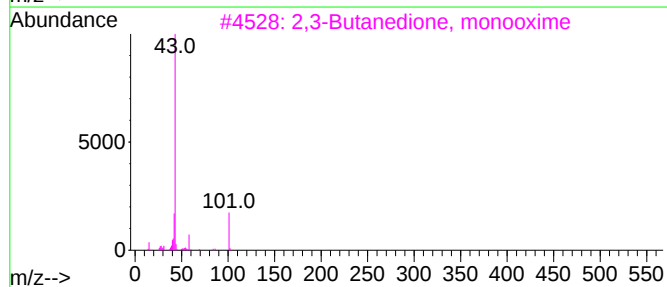
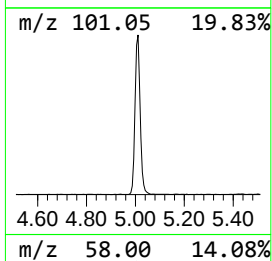
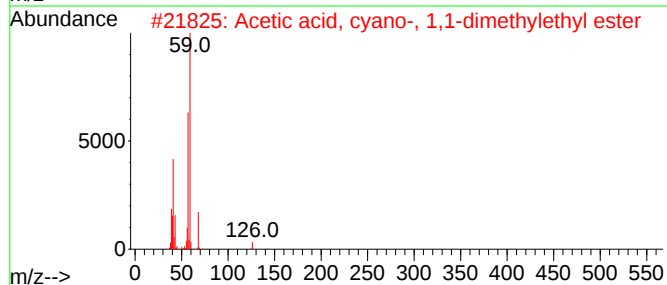
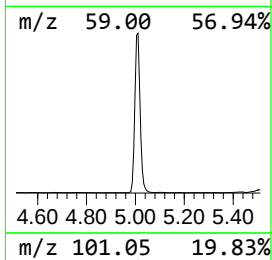
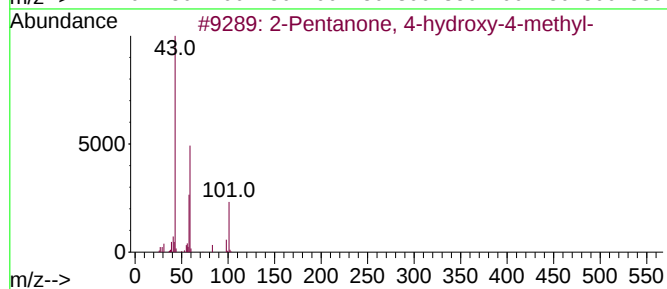
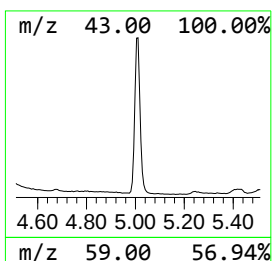
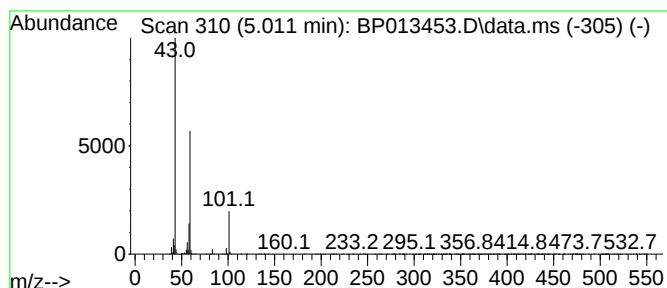
Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.011	28.44 ng	3900360	1,4-Dichlorobenzene-d4			7.922
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-		116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...		141	C7H11NO2	001116-98-9	23
3	2,3-Butanedione, monooxime		101	C4H7NO2	000057-71-6	9
4	Guanidine		59	CH5N3	000113-00-8	9
5	Morpholine, 4-methyl-		101	C5H11NO	000109-02-4	9



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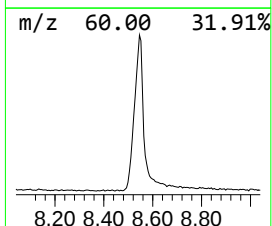
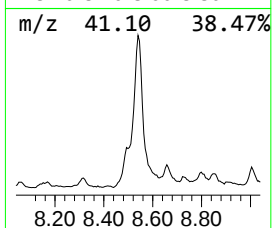
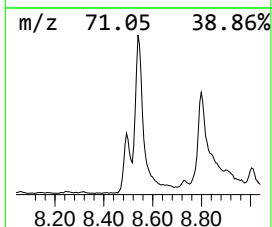
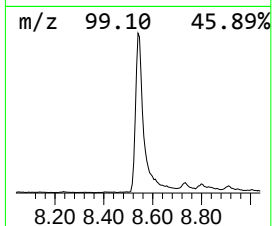
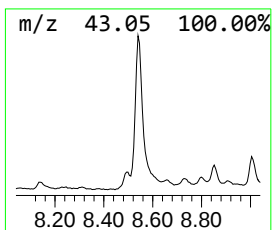
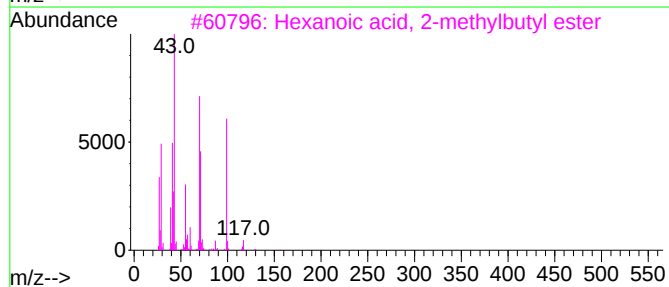
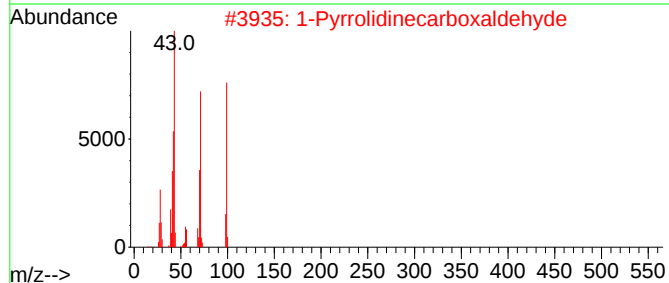
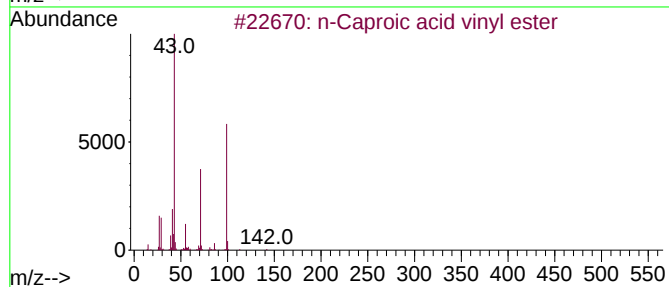
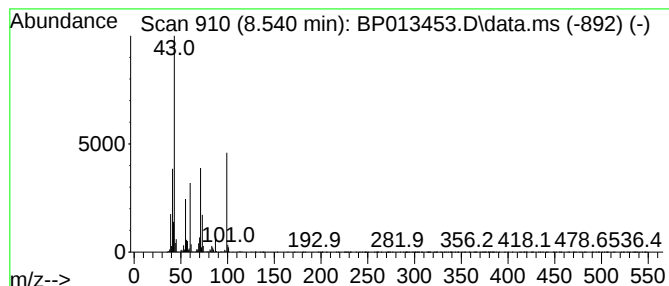
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Caproic acid vinyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
8.540	48.52 ng	6653960	1,4-Dichlorobenzene-d4	7.922	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	53
2	1-Pyrrolidinecarboxaldehyde	99	C5H9NO	003760-54-1	47
3	Hexanoic acid, 2-methylbutyl ester	186	C11H22O2	002601-13-0	45
4	2-Pentene, 5-(pentyloxy)-, (E)-	156	C10H20O	056052-85-8	45
5	Hexanoic acid, propyl ester	158	C9H18O2	000626-77-7	42



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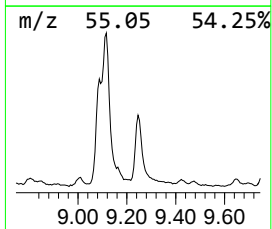
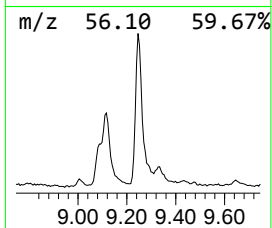
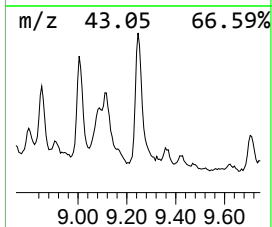
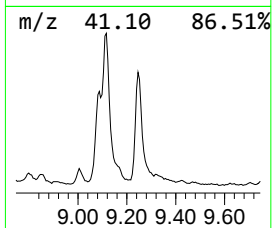
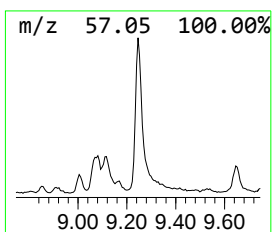
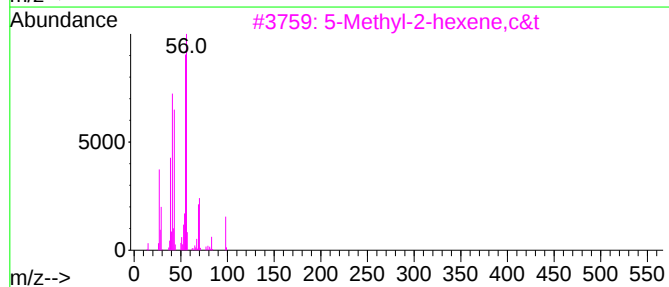
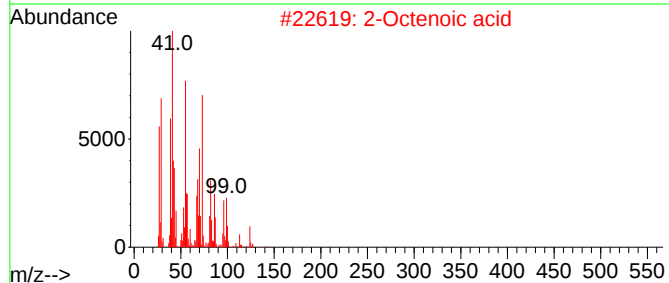
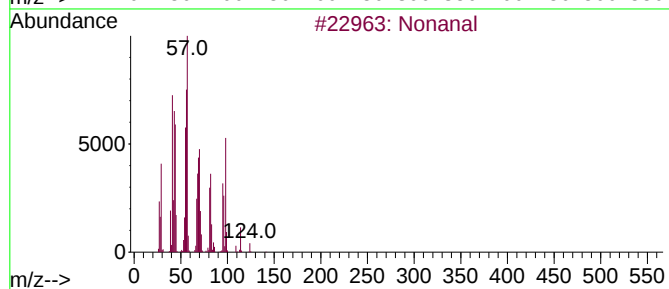
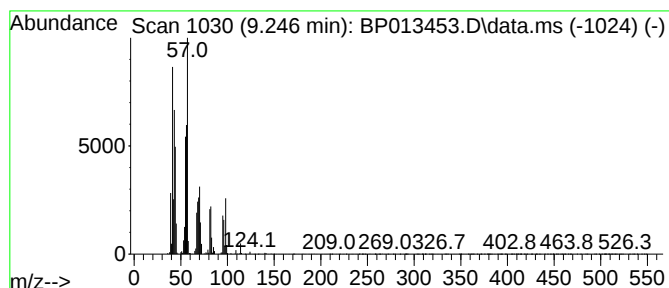
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Nonanal Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.246	20.46 ng	2805450	1,4-Dichlorobenzene-d4	7.922

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	83
2			2-Octenoic acid	142	C8H14O2	001470-50-4	38
3			5-Methyl-2-hexene,c&t	98	C7H14	003404-62-4	30
4			Cyclohexanol, 4-methyl-	114	C7H14O	000589-91-3	27
5			10-Azido-1-decanethiol	215	C10H21N3S	1152113-44-4	27



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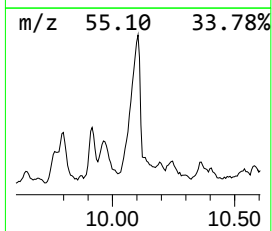
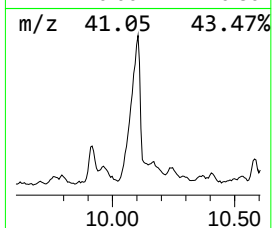
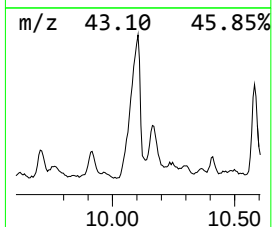
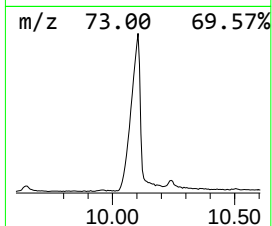
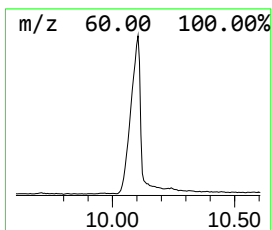
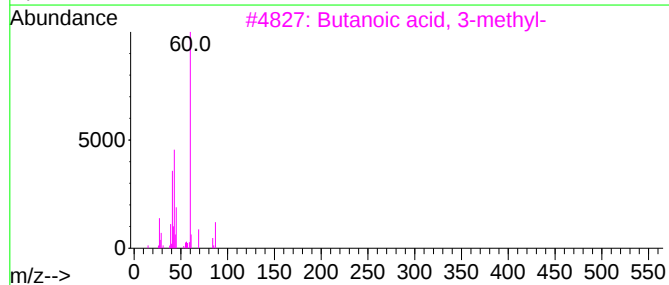
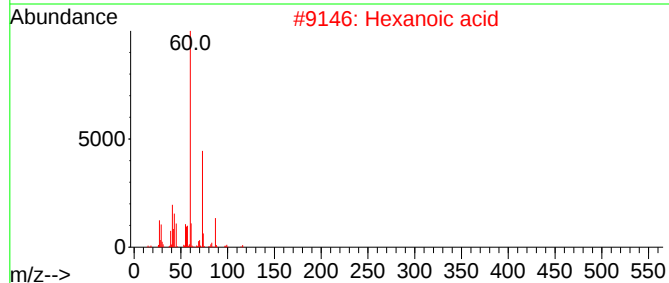
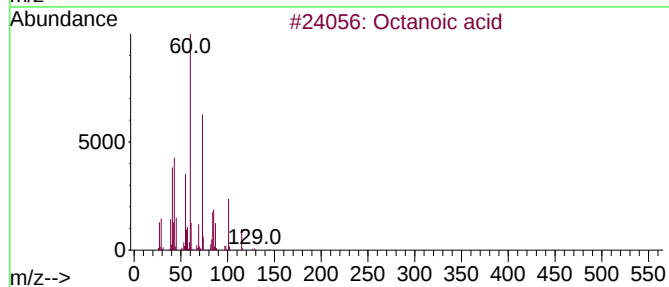
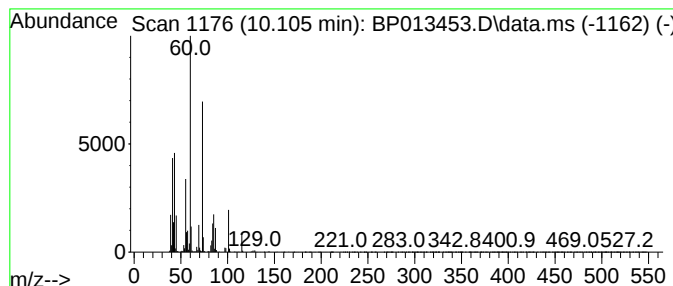
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Octanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.105	22.99 ng	5110940	Naphthalene-d8	10.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octanoic acid	144	C8H16O2	000124-07-2	97
2			Hexanoic acid	116	C6H12O2	000142-62-1	64
3			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	53
4			Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	50
5			Pentanoic acid	102	C5H10O2	000109-52-4	50



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-03

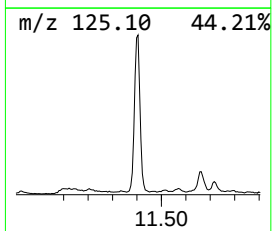
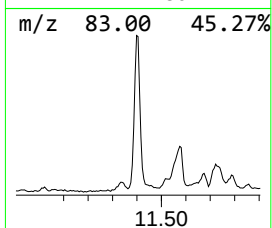
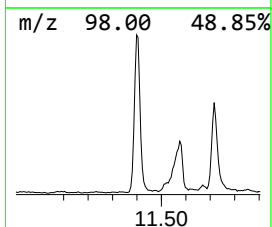
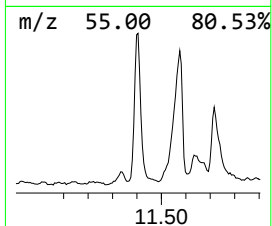
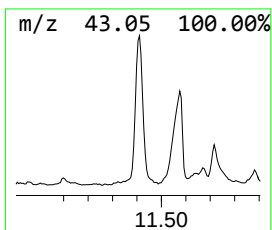
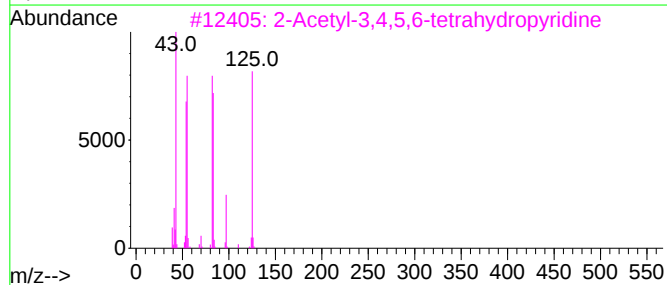
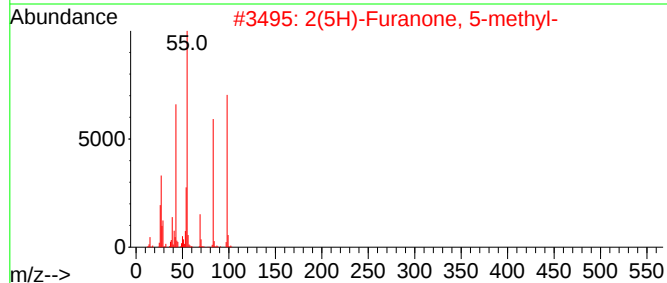
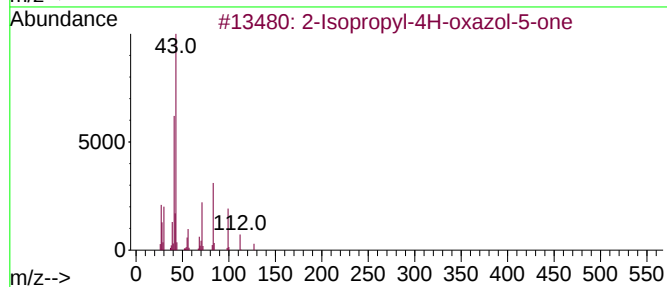
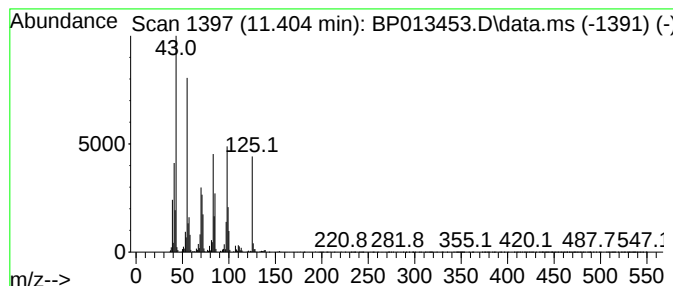
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown11.405 Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.405	16.86 ng	3746610	Naphthalene-d8	10.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2		Isopropyl-4H-oxazol-5-one	127	C6H9N02	1000190-01-9	27
2	2		(5H)-Furanone, 5-methyl-	98	C5H6O2	000591-11-7	27
3	2		Acetyl-3,4,5,6-tetrahydropyridine	125	C7H11N0	027300-27-2	27
4	4		Formaldehyde, methyl(2-propenyl)...	98	C5H10N2	066075-09-0	22
5	5		Diethylcyanamide	98	C5H10N2	000617-83-4	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
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Sample : 01064-08
Misc :
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Instrument :
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ClientSampleId :
S-14-03

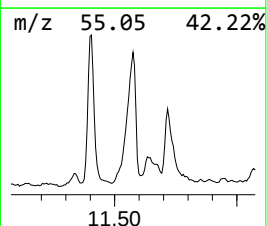
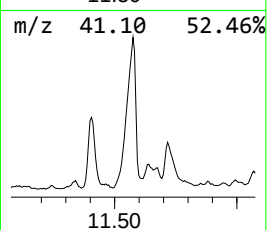
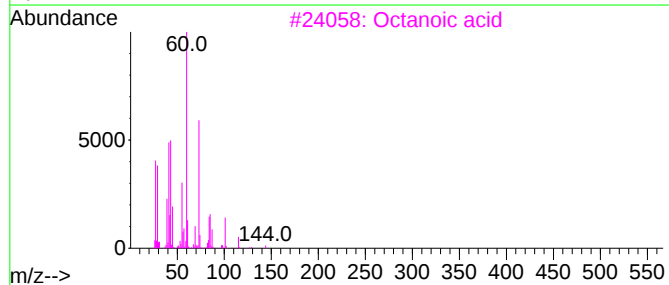
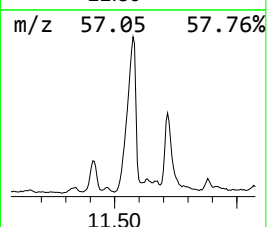
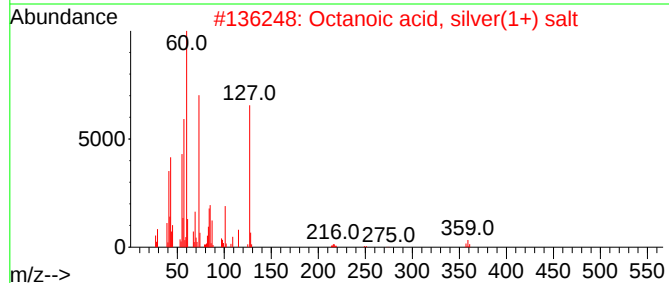
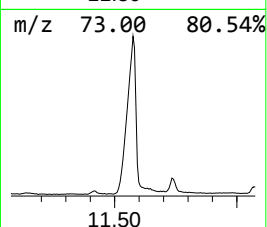
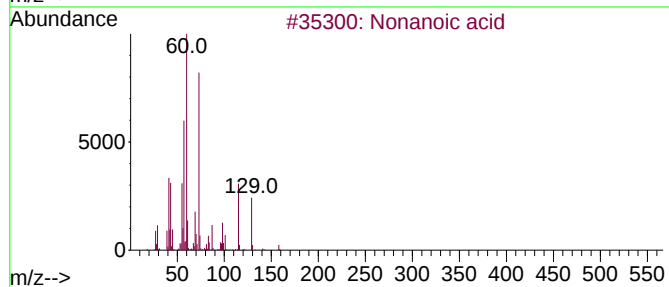
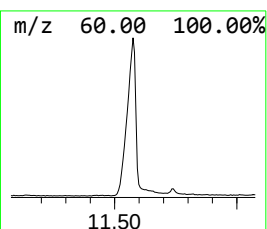
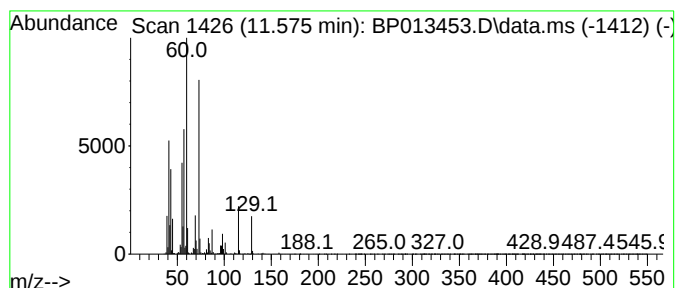
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.575	32.23 ng	7163350	Naphthalene-d8	10.734

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanoic acid	158	C9H18O2	000112-05-0	95
2			Octanoic acid, silver(1+) salt	250	C8H15AgO2	024927-67-1	58
3			Octanoic acid	144	C8H16O2	000124-07-2	50
4			Hexanoic acid	116	C6H12O2	000142-62-1	50
5			Pentanoic acid	102	C5H10O2	000109-52-4	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
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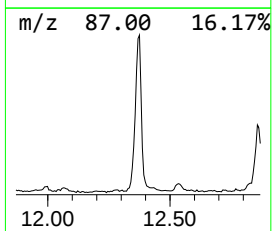
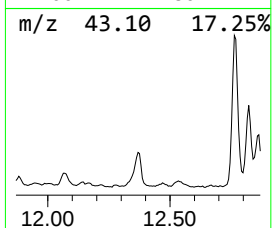
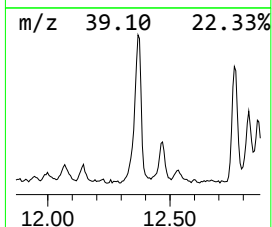
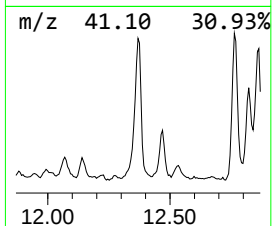
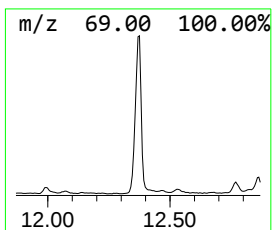
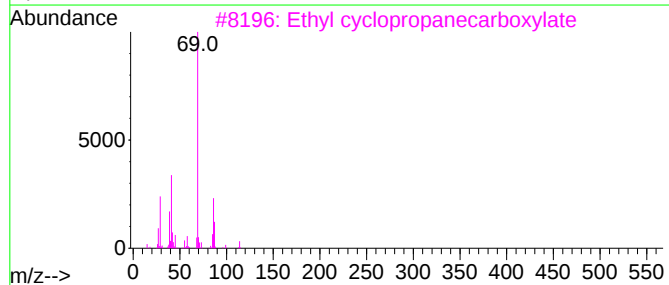
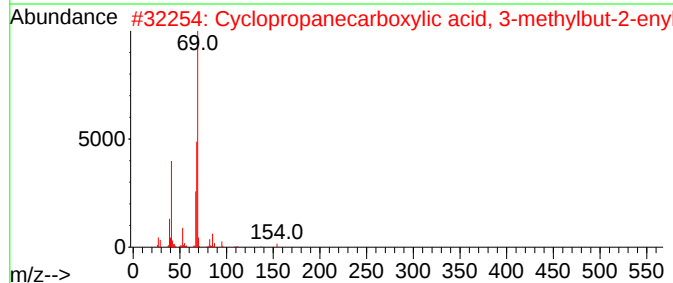
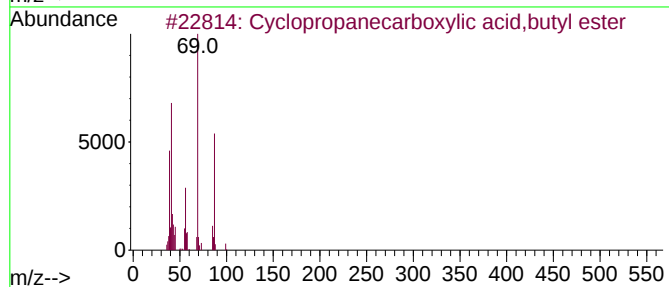
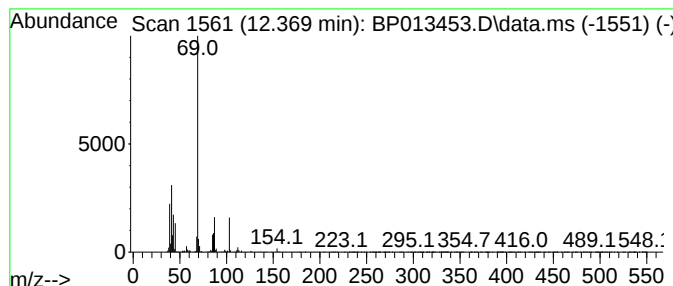
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Cyclopropanecarboxylic acid... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.369	13.62 ng	3027030	Naphthalene-d8	10.734	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	53
2	Cyclopropanecarboxylic acid, 3-m...	154	C9H14O2	1000299-37-4	53
3	Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	38
4	Cyclopropanecarboxylic acid, 2-m...	170	C10H18O2	1000354-65-8	36
5	Vinyl crotonate	112	C6H8O2	014861-06-4	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
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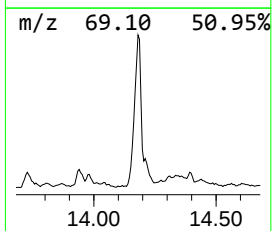
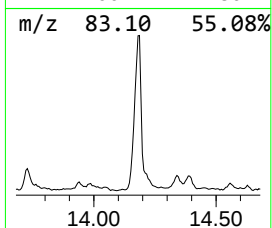
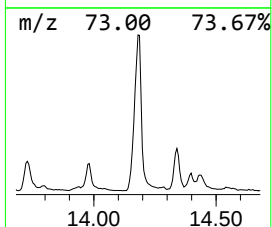
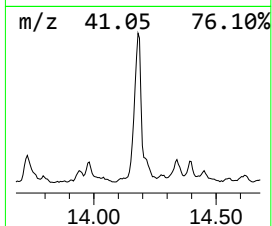
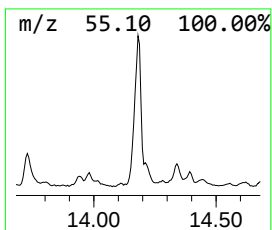
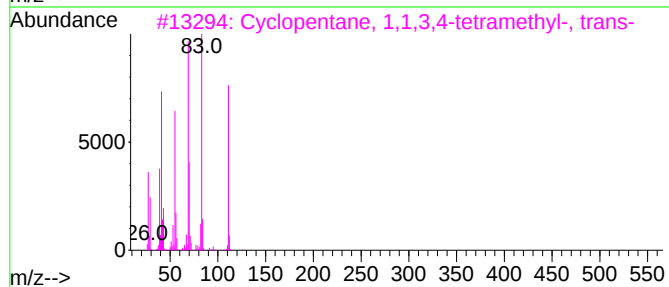
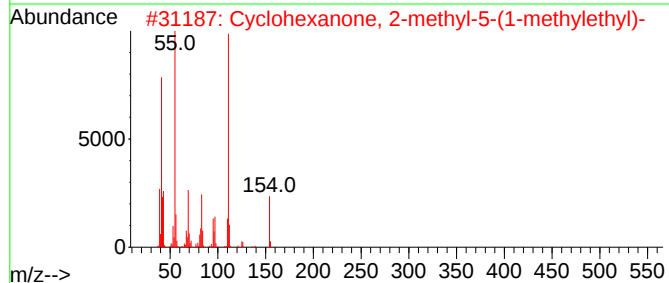
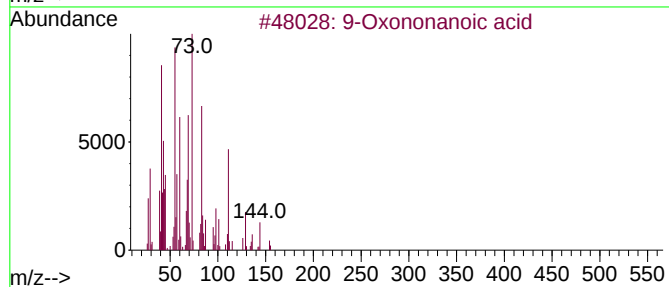
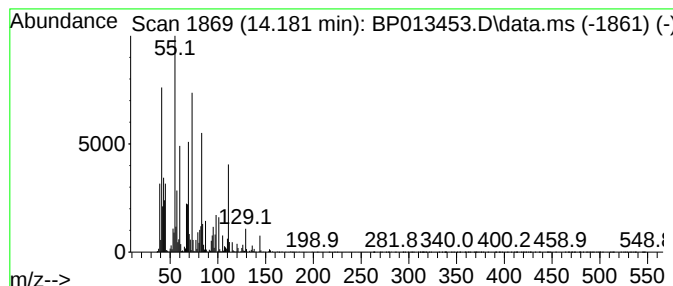
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 9-Oxononanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.181	19.30 ng	6312680	Acenaphthene-d10	14.569	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Oxononanoic acid	172	C9H16O3	002553-17-5	91
2	Cyclohexanone, 2-methyl-5-(1-met...	154	C10H18O	059471-80-6	35
3	Cyclopentane, 1,1,3,4-tetramethy...	126	C9H18	020309-77-7	35
4	Cyclohexanecarboxylic acid, ethe...	154	C9H14O2	004840-76-0	30
5	Cyclobutanecarboxylic acid, prop...	142	C8H14O2	1000280-40-0	22



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
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Misc :
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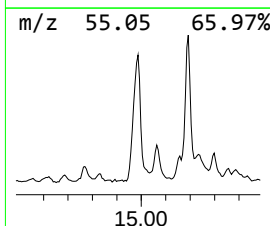
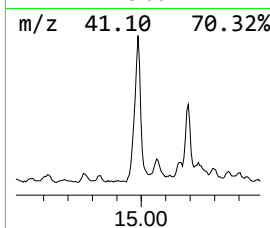
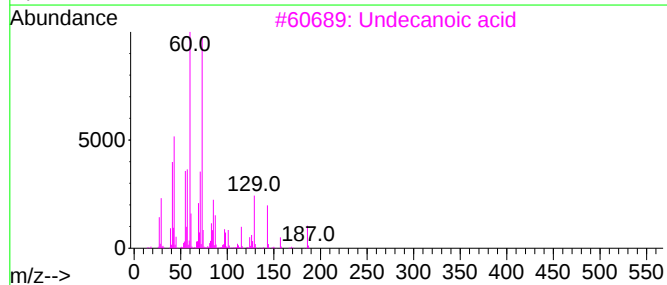
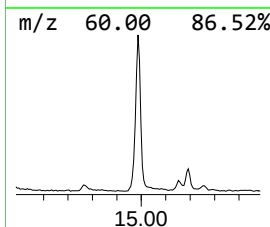
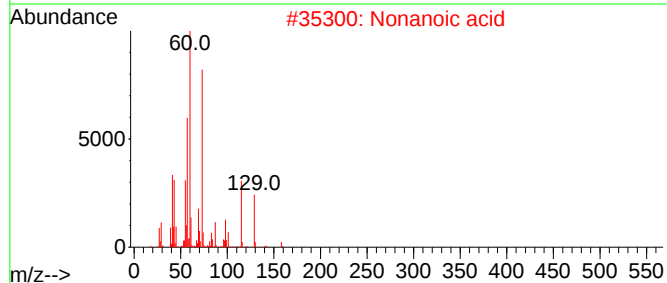
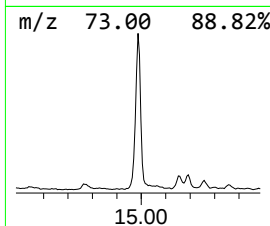
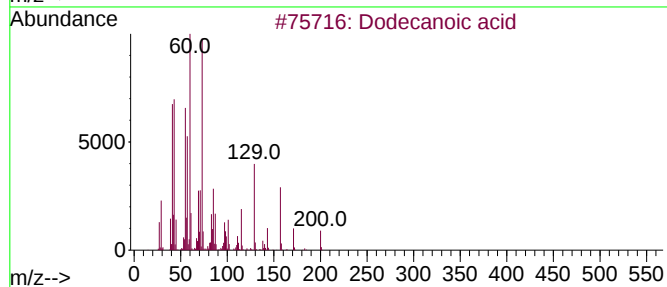
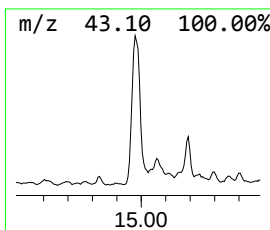
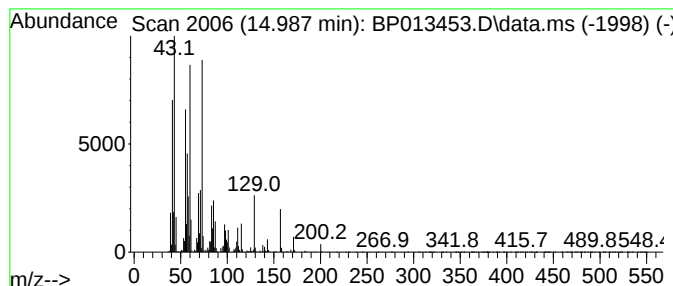
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Dodecanoic acid Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD		R.T.	
14.987	18.70 ng	6116620	Acenaphthene-d10		14.569	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dodecanoic acid		200	C12H24O2	000143-07-7	97
2	Nonanoic acid		158	C9H18O2	000112-05-0	86
3	Undecanoic acid		186	C11H22O2	000112-37-8	80
4	n-Decanoic acid		172	C10H20O2	000334-48-5	53
5	Octanoic acid		144	C8H16O2	000124-07-2	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
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ALS Vial : 16 Sample Multiplier: 1

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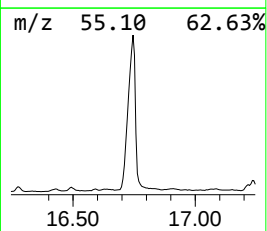
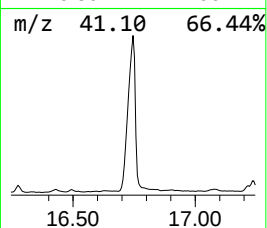
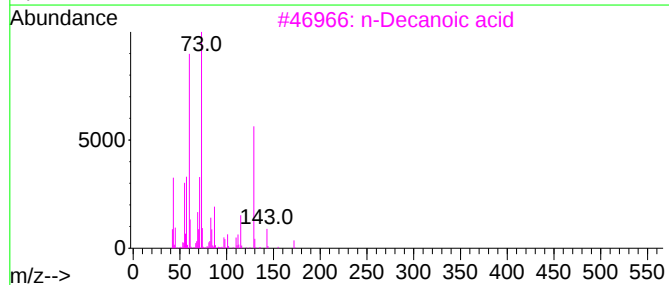
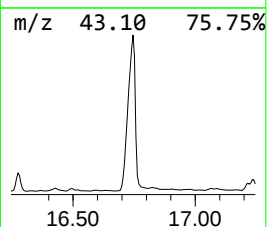
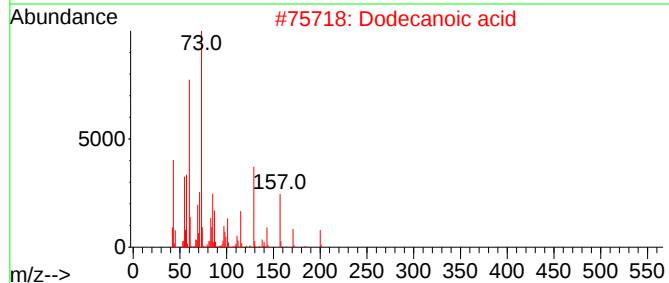
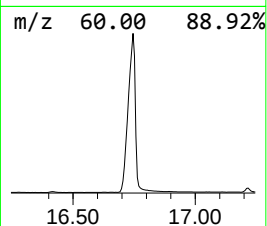
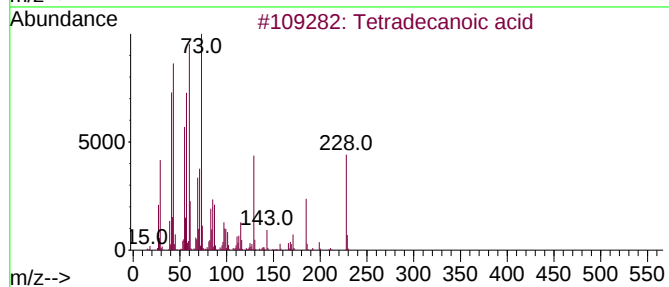
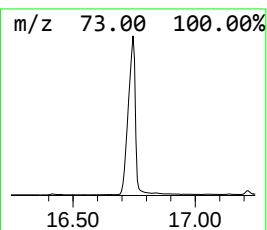
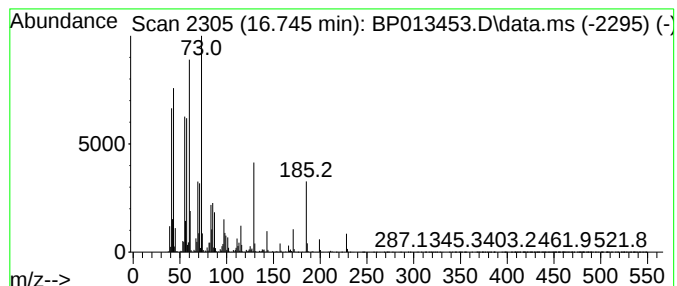
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Tetradecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.745	107.05 ng	45012100	Phenanthrene-d10	17.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
2			Dodecanoic acid	200	C12H24O2	000143-07-7	83
3			n-Decanoic acid	172	C10H20O2	000334-48-5	70
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Undecanoic acid	186	C11H22O2	000112-37-8	58



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

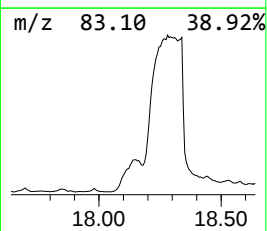
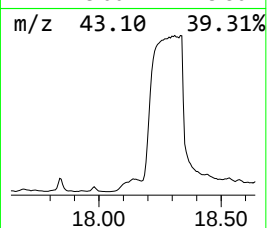
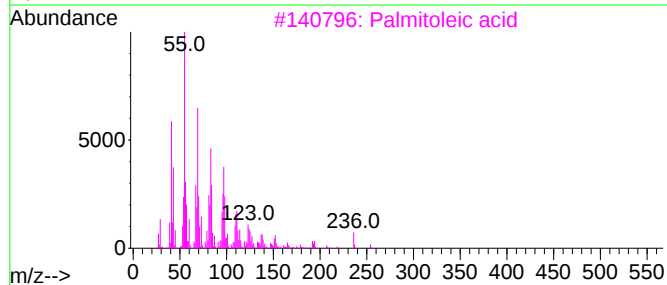
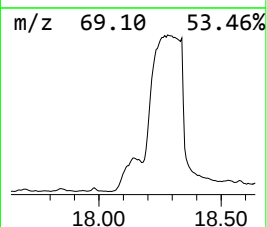
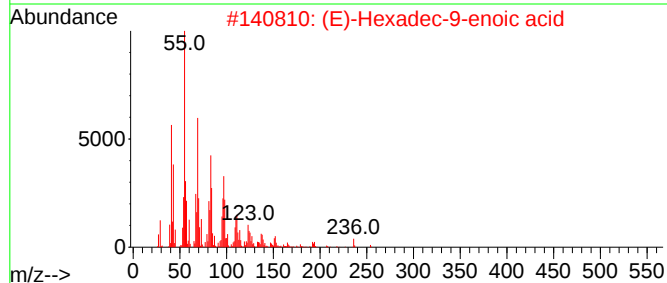
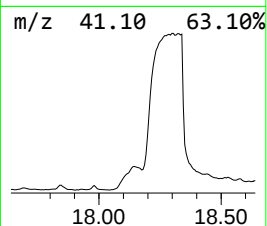
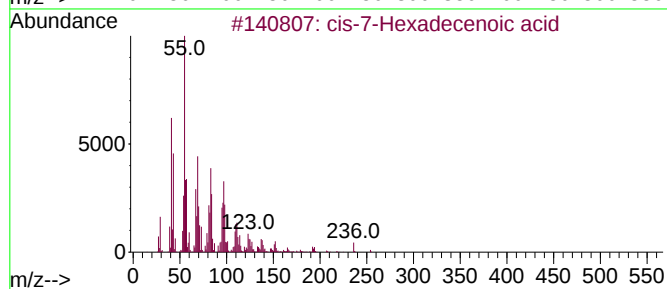
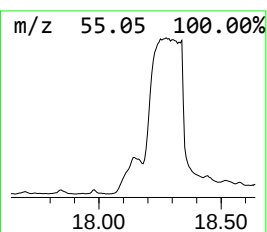
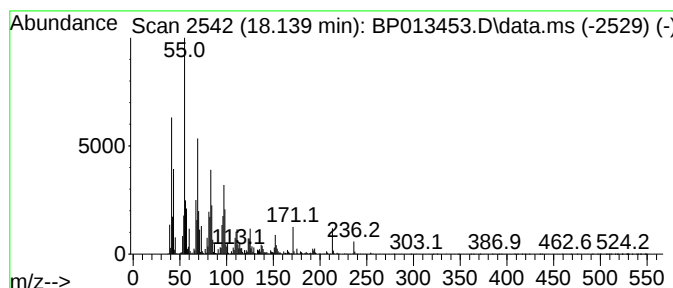
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BNA_P
ClientSampleId :
S-14-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 cis-7-Hexadecenoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.139	47.75 ng	20078800	Phenanthrene-d10		17.328	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	cis-7-Hexadecenoic acid		254	C16H30O2	002416-19-5	99
2	(E)-Hexadec-9-enoic acid		254	C16H30O2	010030-73-6	99
3	Palmitoleic acid		254	C16H30O2	000373-49-9	90
4	9-Hexadecenoic acid		254	C16H30O2	002091-29-4	81
5	Oxacycloheptadecan-2-one		254	C16H30O2	000109-29-5	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-03

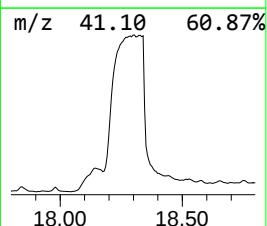
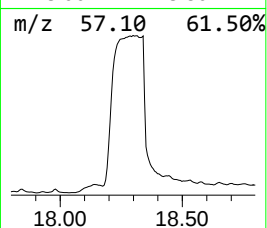
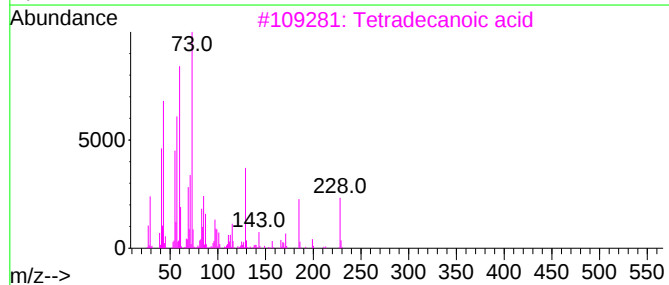
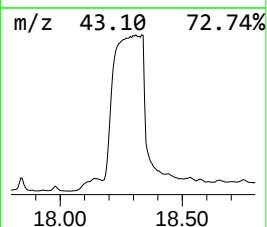
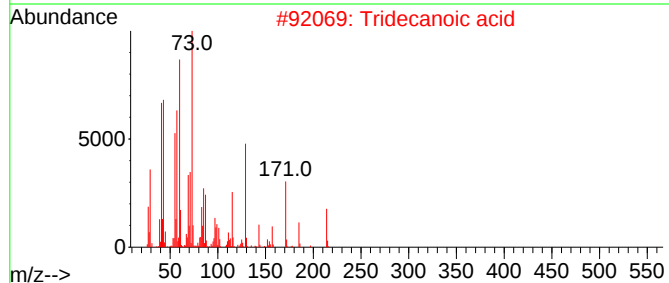
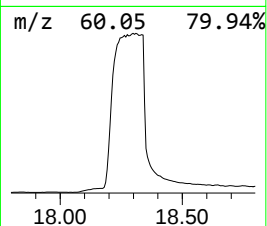
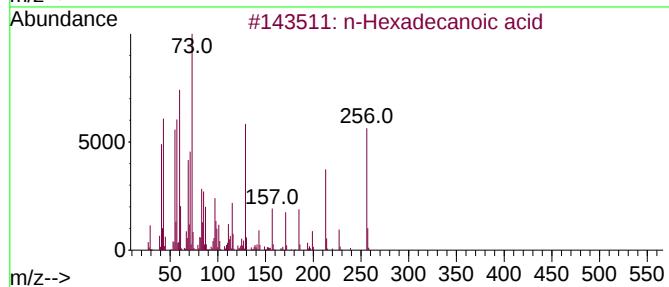
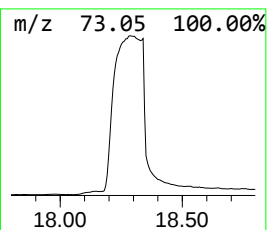
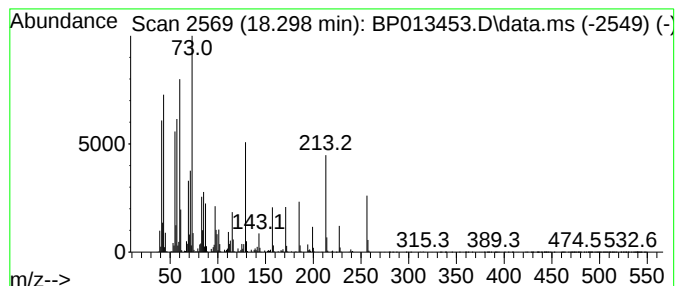
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.298	597.80 ng	251362000	Phenanthrene-d10	17.328

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2		Tridecanoic acid	214	C13H26O2	000638-53-9	92
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	52
5		Undecanoic acid	186	C11H22O2	000112-37-8	45



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-03

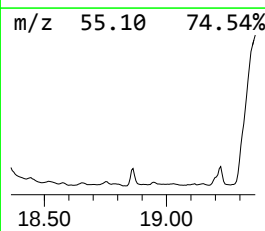
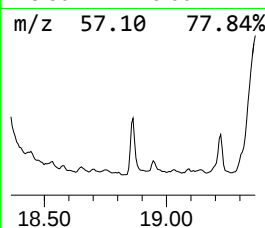
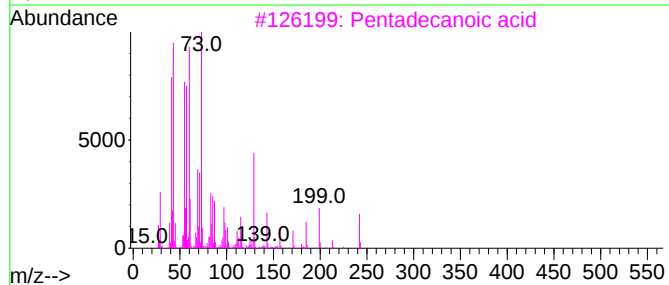
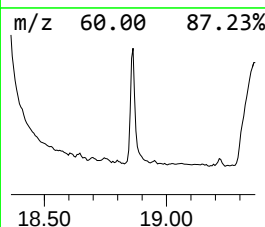
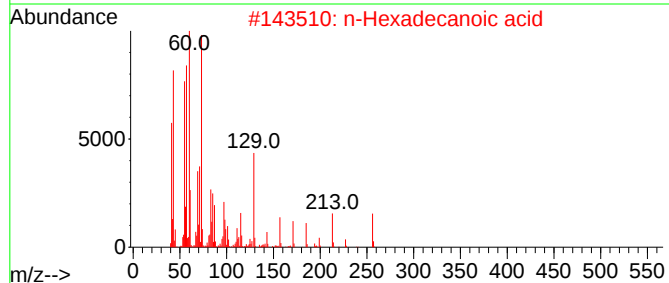
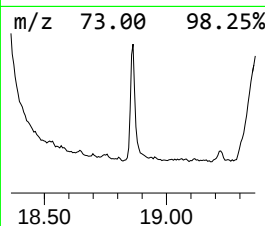
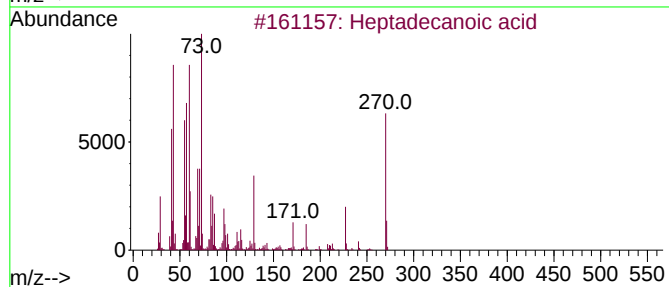
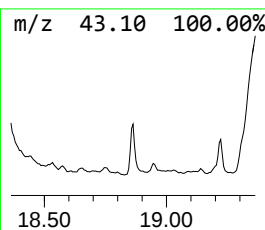
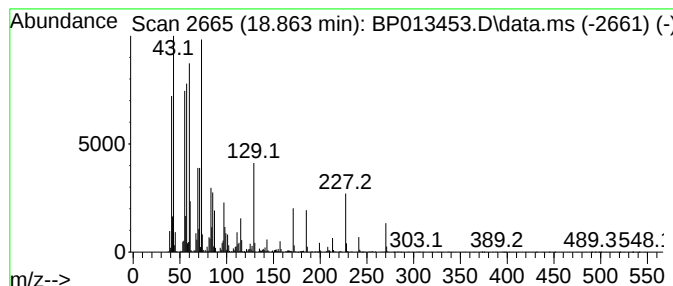
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Heptadecanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.863	14.93 ng	6275720	Phenanthrene-d10	17.328

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecanoic acid	270	C17H34O2	000506-12-7	93
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			Tridecanoic acid	214	C13H26O2	000638-53-9	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
S-14-03

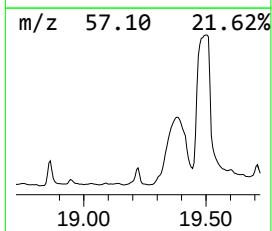
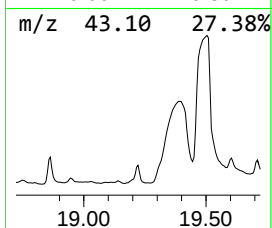
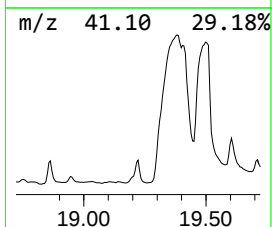
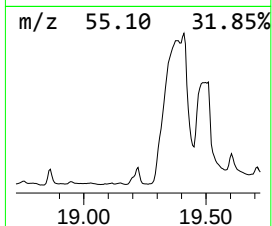
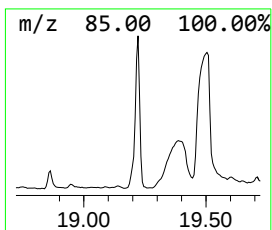
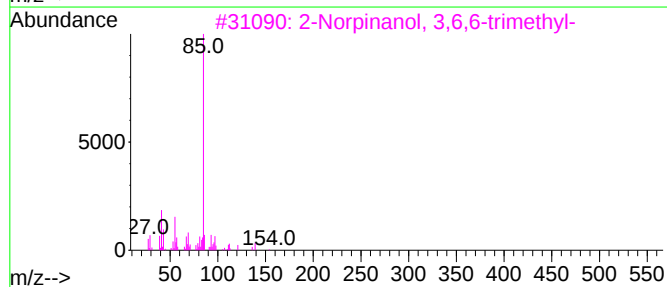
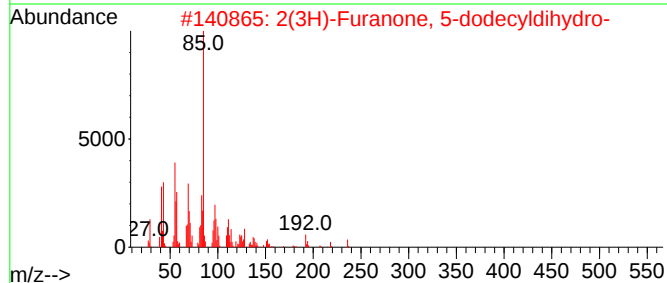
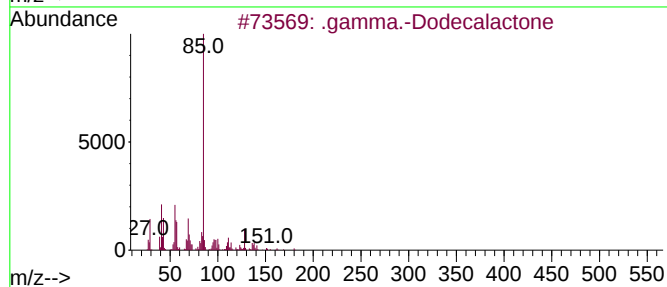
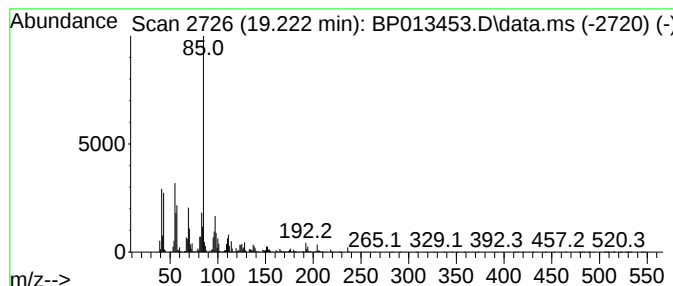
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 .gamma.-Dodecalactone Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.222	17.27 ng	7263250	Phenanthrene-d10	17.328

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.gamma.-Dodecalactone	198	C12H22O2	002305-05-7	72
2		2(3H)-Furanone, 5-dodecyldihydro-	254	C16H30O2	000730-46-1	64
3		2-Norpinanol, 3,6,6-trimethyl-	154	C10H18O	029548-09-2	59
4		10-Methylundecan-4-olide	198	C12H22O2	1000370-40-5	59
5		Valeric acid, undec-2-enyl ester	254	C16H30O2	1000292-49-1	53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

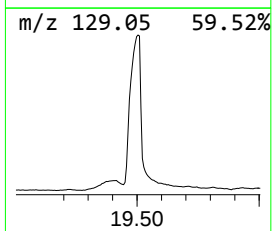
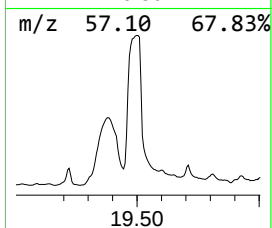
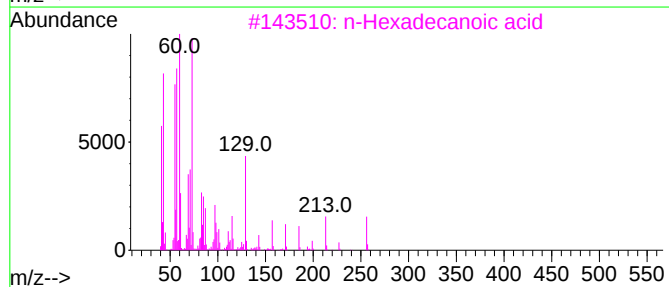
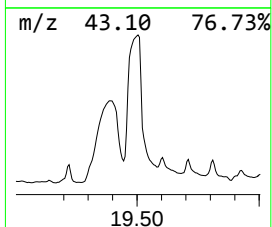
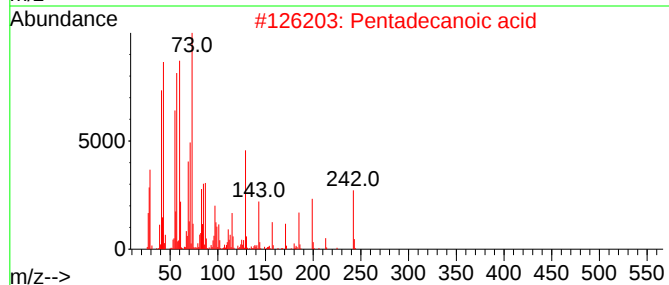
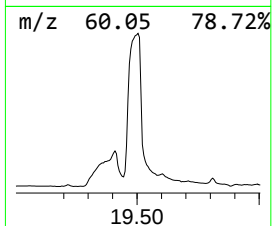
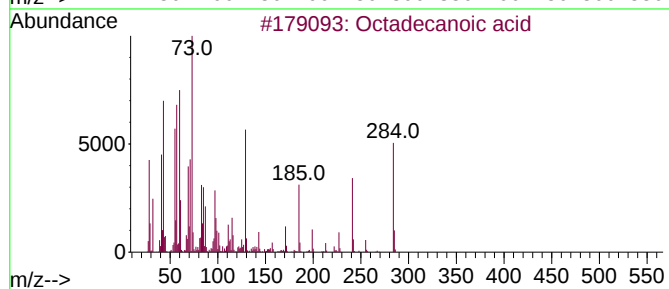
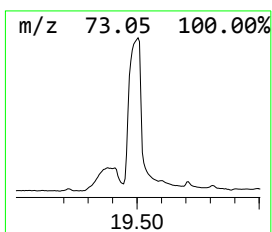
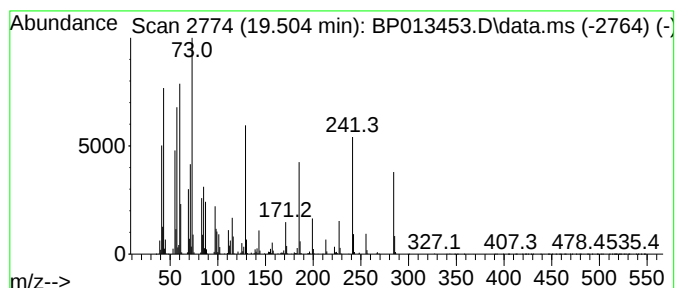
Instrument :
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ClientSampleId :
S-14-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.504	154.29 ng	112666000	Chrysene-d12	21.422
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 83
3		n-Hexadecanoic acid	256 C16H32O2	000057-10-3 83
4		Tetradecanoic acid	228 C14H28O2	000544-63-8 72
5		Tridecanoic acid	214 C13H26O2	000638-53-9 53



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
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Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

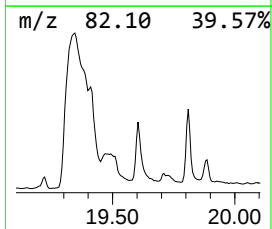
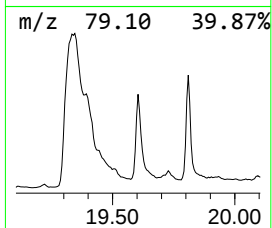
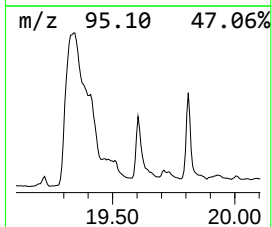
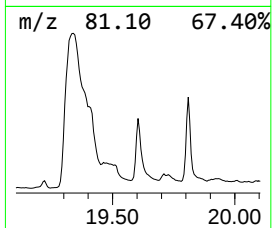
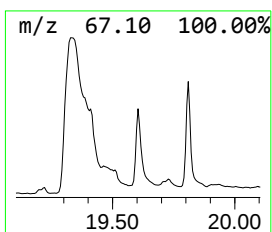
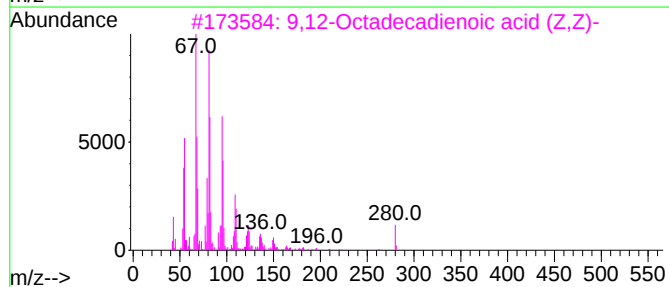
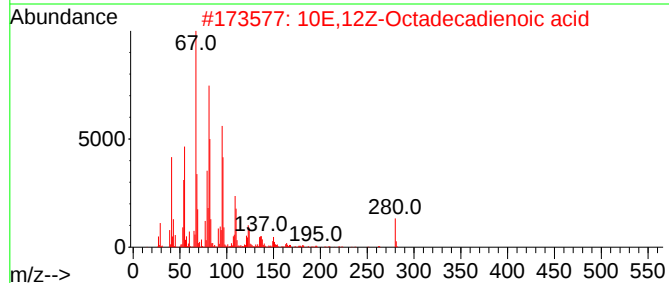
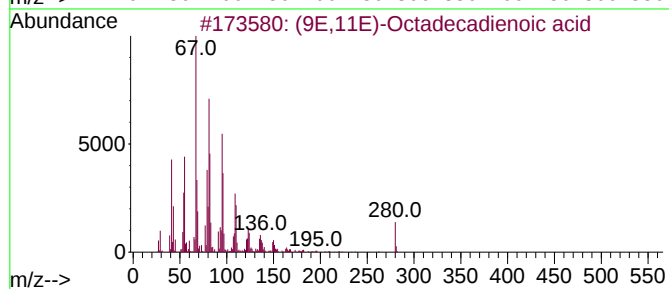
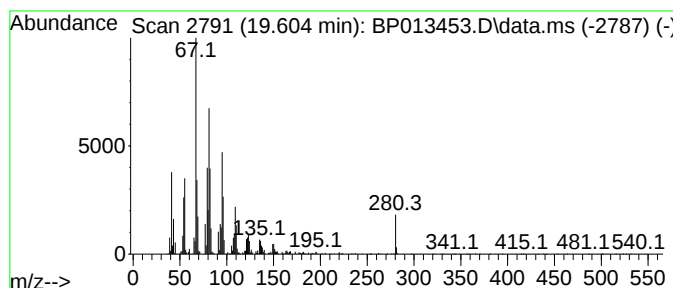
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 (9E,11E)-Octadecadienoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.604	17.90 ng	13073200	Chrysene-d12	21.422
Hit#	of 5	Tentative ID	MW MolForm	CAS# Qual
1		(9E,11E)-Octadecadienoic acid	280 C18H32O2	000544-71-8 99
2		10E,12Z-Octadecadienoic acid	280 C18H32O2	002420-56-6 98
3		9,12-Octadecadienoic acid (Z,Z)-	280 C18H32O2	000060-33-3 96
4		9,12-Octadecadien-1-ol, (Z,Z)-	266 C18H34O	000506-43-4 91
5		3,4-Octadiene, 7-methyl-	124 C9H16	037050-05-8 81



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

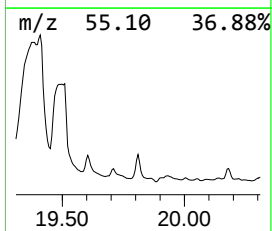
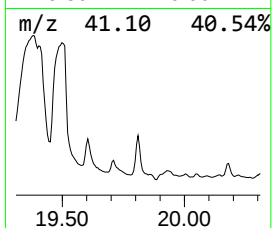
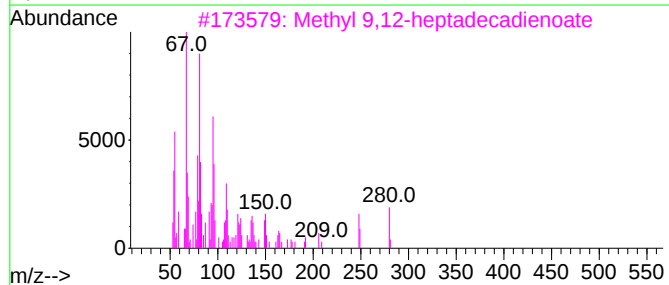
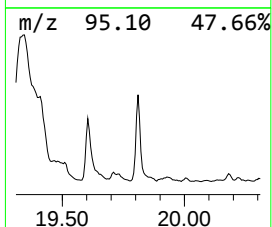
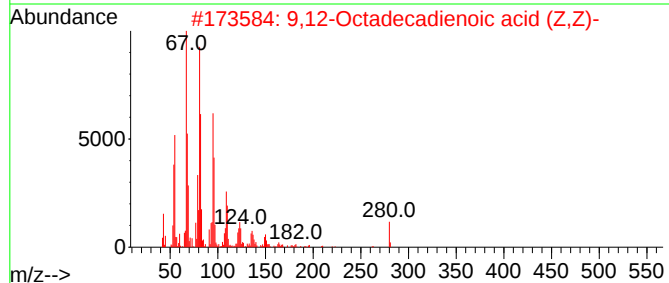
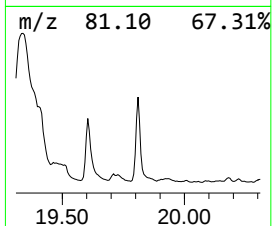
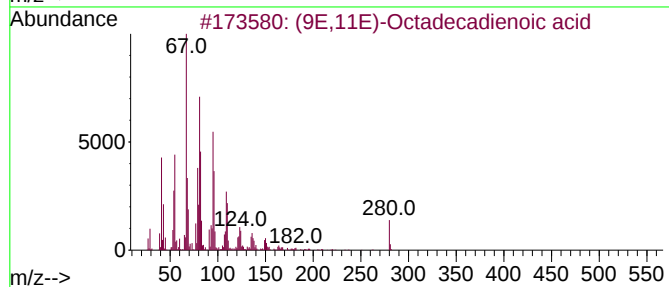
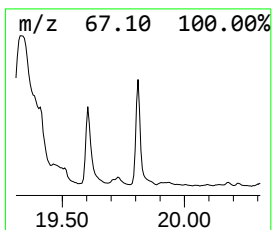
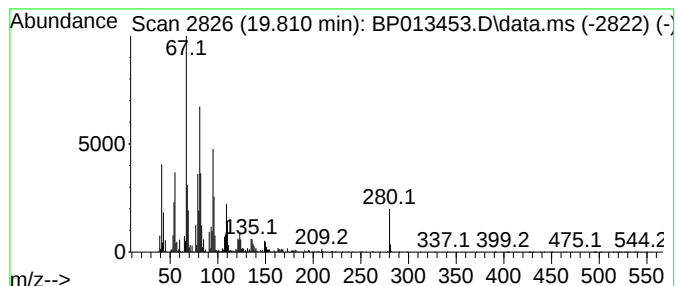
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S-14-03

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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 18 9,12-Octadecadienoic acid (... Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.810	17.70 ng	12927700	Chrysene-d12	21.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(9E,11E)-Octadecadienoic acid	280	C18H32O2	000544-71-8	99
2	9,12-Octadecadienoic acid (Z,Z)-	280	C18H32O2	000060-33-3	95
3	Methyl 9,12-heptadecadienoate	280	C18H32O2	1000336-36-2	81
4	10E,12Z-Octadecadienoic acid	280	C18H32O2	002420-56-6	64
5	1,E-11,Z-13-Octadecatriene	248	C18H32	080625-36-1	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

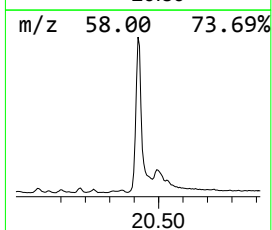
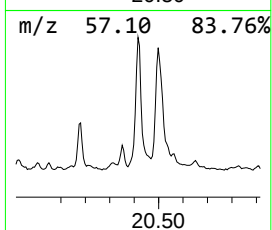
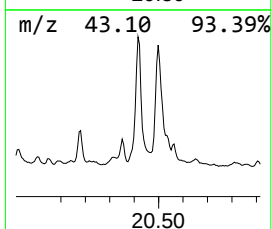
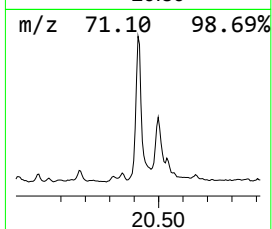
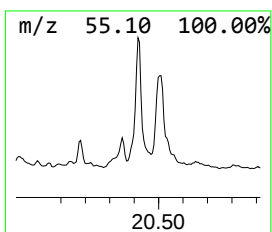
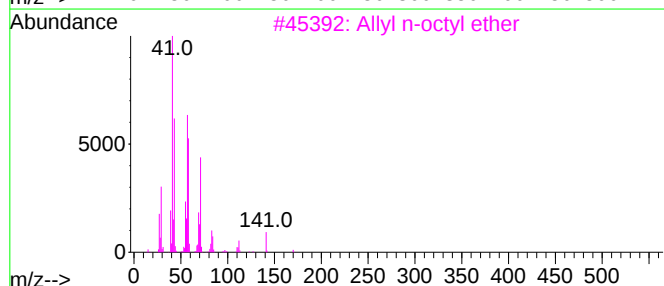
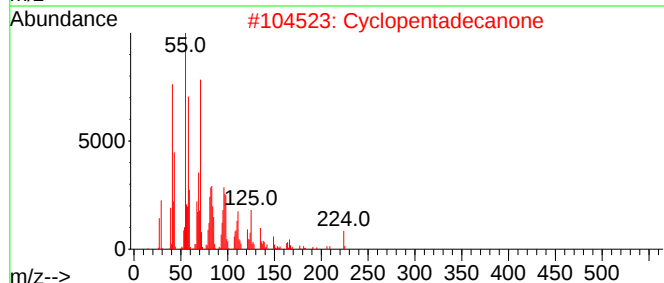
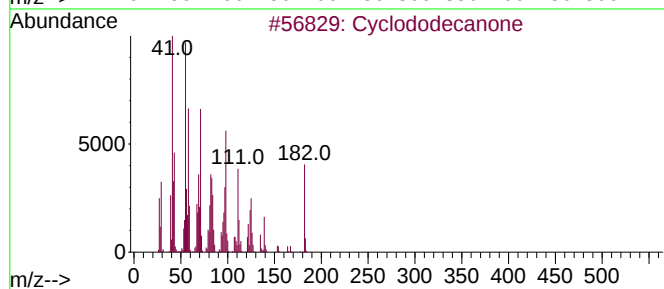
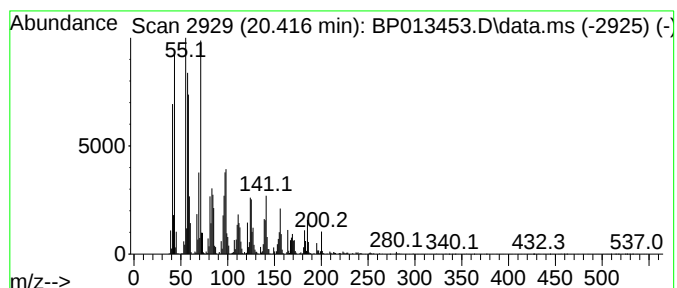
Instrument :
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ClientSampleId :
S-14-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Cyclododecanone Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.416	33.24 ng	24274700	Chrysene-d12	21.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclododecanone	182	C12H22O	000830-13-7	86
2	Cyclopentadecanone	224	C15H28O	000502-72-7	62
3	Allyl n-octyl ether	170	C11H22O	003295-97-4	45
4	9-Octadecanone	268	C18H36O	018394-00-8	45
5	5-Decanone, 2-methyl-	170	C11H22O	054410-89-8	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
Data File : BP013453.D
Acq On : 11 Jan 2023 20:29
Operator : CG/JU
Sample : 01064-08
Misc :
ALS Vial : 16 Sample Multiplier: 1

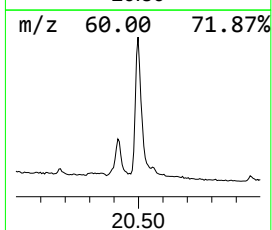
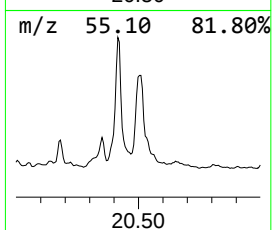
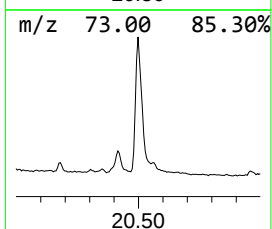
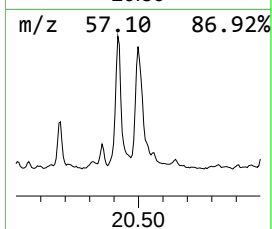
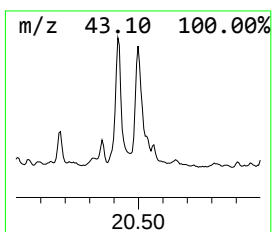
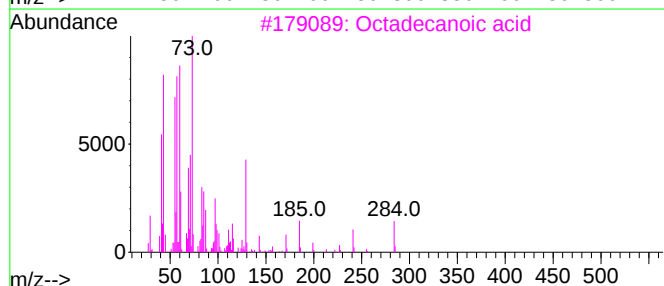
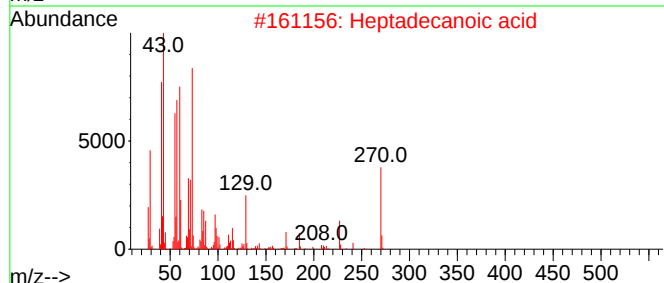
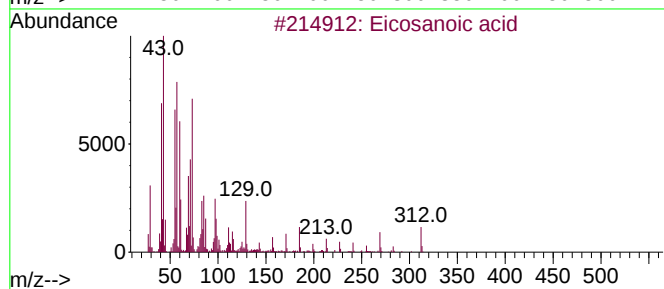
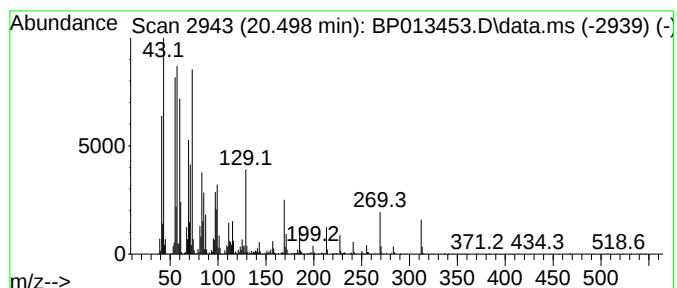
Instrument :
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ClientSampleId :
S-14-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Eicosanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
20.498	32.68 ng	23865700	Chrysene-d12	21.422	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosanoic acid	312	C20H40O2	000506-30-9	99
2	Heptadecanoic acid	270	C17H34O2	000506-12-7	70
3	Octadecanoic acid	284	C18H36O2	000057-11-4	55
4	Tridecanoic acid	214	C13H26O2	000638-53-9	49
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	49



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP011123\
 Data File : BP013453.D
 Acq On : 11 Jan 2023 20:29
 Operator : CG/JU
 Sample : 01064-08
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 S-14-03

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP121322.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
Hexanal	4.434	94.5	ng	12964000	1	7.922	2742530	20.0
2-Pentanone, 4-...	5.011	28.4	ng	3900360	1	7.922	2742530	20.0
n-Caproic acid ...	8.540	48.5	ng	6653960	1	7.922	2742530	20.0
Nonanal	9.246	20.5	ng	2805450	1	7.922	2742530	20.0
Octanoic acid	10.105	23.0	ng	5110940	2	10.734	4445490	20.0
unknown11.405	11.405	16.9	ng	3746610	2	10.734	4445490	20.0
Nonanoic acid	11.575	32.2	ng	7163350	2	10.734	4445490	20.0
Cyclopropanecar...	12.369	13.6	ng	3027030	2	10.734	4445490	20.0
9-Oxononanoic acid	14.181	19.3	ng	6312680	3	14.569	6542210	20.0
Dodecanoic acid	14.987	18.7	ng	6116620	3	14.569	6542210	20.0
Tetradecanoic acid	16.745	107.1	ng	45012100	4	17.328	8409590	20.0
cis-7-Hexadecen...	18.139	47.8	ng	20078800	4	17.328	8409590	20.0
n-Hexadecanoic ...	18.298	597.8	ng	251362000	4	17.328	8409590	20.0
Heptadecanoic acid	18.863	14.9	ng	6275720	4	17.328	8409590	20.0
.gamma.-Dodecal...	19.222	17.3	ng	7263250	4	17.328	8409590	20.0
Octadecanoic acid	19.504	154.3	ng	112666000	5	21.422	14604500	20.0
(9E,11E)-Octade...	19.604	17.9	ng	13073200	5	21.422	14604500	20.0
9,12-Octadecadi...	19.810	17.7	ng	12927700	5	21.422	14604500	20.0
Cyclododecanone	20.416	33.2	ng	24274700	5	21.422	14604500	20.0
Eicosanoic acid	20.498	32.7	ng	23865700	5	21.422	14604500	20.0