

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
 Data File : BP020615.D
 Acq On : 13 Jun 2024 17:22
 Operator : MA/JU
 Sample : P2855-05
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 72-11989

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-BP052924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020615.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.023	3	6	22	rVB	1937520	2757618	28.29%	4.666%
2	3.552	92	96	106	rVB	190107	261219	2.68%	0.442%
3	4.922	320	329	337	rVB2	162763	272386	2.79%	0.461%
4	5.370	397	405	414	rBV	2591844	4109978	42.17%	6.954%
5	6.934	662	671	691	rBV	2635734	4200180	43.09%	7.107%
6	7.746	800	809	816	rBV	724786	1229740	12.62%	2.081%
7	8.899	997	1005	1023	rBV	1500848	2757806	28.29%	4.666%
8	9.452	1093	1099	1106	rVB	91117	131363	1.35%	0.222%
9	10.299	1236	1243	1256	rBV	124690	267685	2.75%	0.453%
10	10.522	1271	1281	1287	rBV	1004728	1700130	17.44%	2.877%
11	11.257	1397	1406	1427	rBV	141124	309526	3.18%	0.524%
12	12.981	1691	1699	1709	rBV	4208372	6568175	67.39%	11.114%
13	14.375	1928	1936	1943	rBV	1556967	2285892	23.45%	3.868%
14	14.440	1943	1947	1955	rVB	58537	98515	1.01%	0.167%
15	14.598	1966	1974	1980	rBV2	107373	228603	2.35%	0.387%
16	15.892	2186	2194	2213	rBV	3113396	5264694	54.01%	8.908%
17	17.181	2405	2413	2417	rBV	2024454	2791352	28.64%	4.723%
18	17.216	2417	2419	2426	rVV	644683	867417	8.90%	1.468%
19	17.310	2430	2435	2442	rVB	88298	173466	1.78%	0.294%
20	17.487	2458	2465	2475	rBV	150093	248718	2.55%	0.421%
21	17.598	2481	2484	2496	rVB	66883	107726	1.11%	0.182%
22	18.081	2561	2566	2569	rBV	73643	111113	1.14%	0.188%
23	18.128	2569	2574	2582	rVV2	793649	1227227	12.59%	2.077%
24	18.286	2596	2601	2605	rBV	108202	200343	2.06%	0.339%
25	19.039	2725	2729	2734	rBV2	56761	103075	1.06%	0.174%
26	19.310	2770	2775	2782	rBV	907743	1426996	14.64%	2.415%
27	19.457	2796	2800	2807	rBV3	360046	550899	5.65%	0.932%
28	19.657	2830	2834	2835	rBV	160039	177915	1.83%	0.301%
29	19.692	2835	2840	2845	rVB	773916	1142695	11.72%	1.934%
30	19.910	2871	2877	2887	rVB	6790149	9747143	100.00%	16.493%
31	20.210	2926	2928	2933	rVB2	93207	125489	1.29%	0.212%
32	20.316	2943	2946	2949	rBV	89033	107288	1.10%	0.182%
33	21.322	3112	3117	3129	rVB3	474632	998541	10.24%	1.690%
34	21.633	3161	3170	3175	rBV2	1733432	3591279	36.84%	6.077%
35	24.974	3731	3738	3748	rVB2	1083843	2956907	30.34%	5.003%

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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-BP052924.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

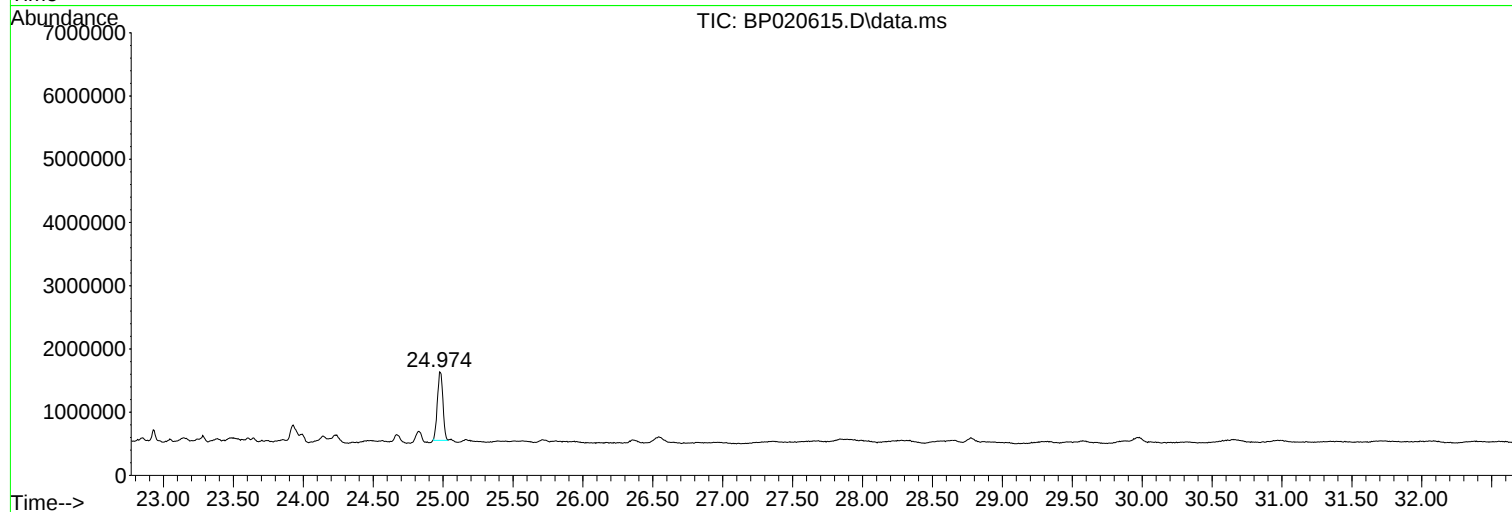
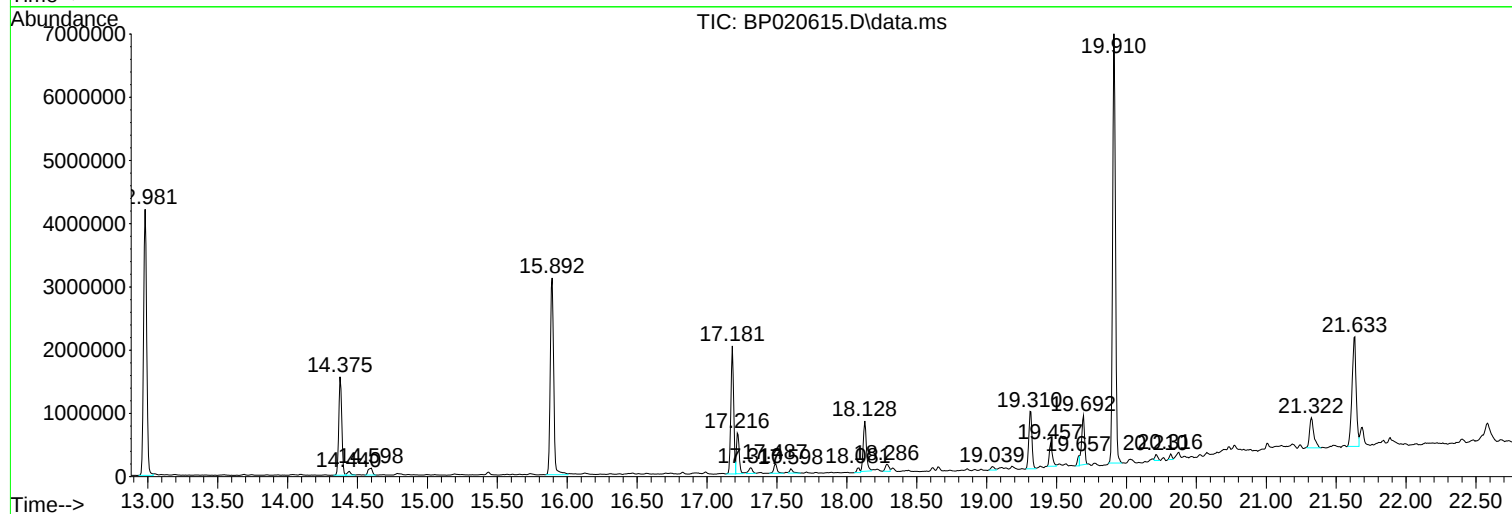
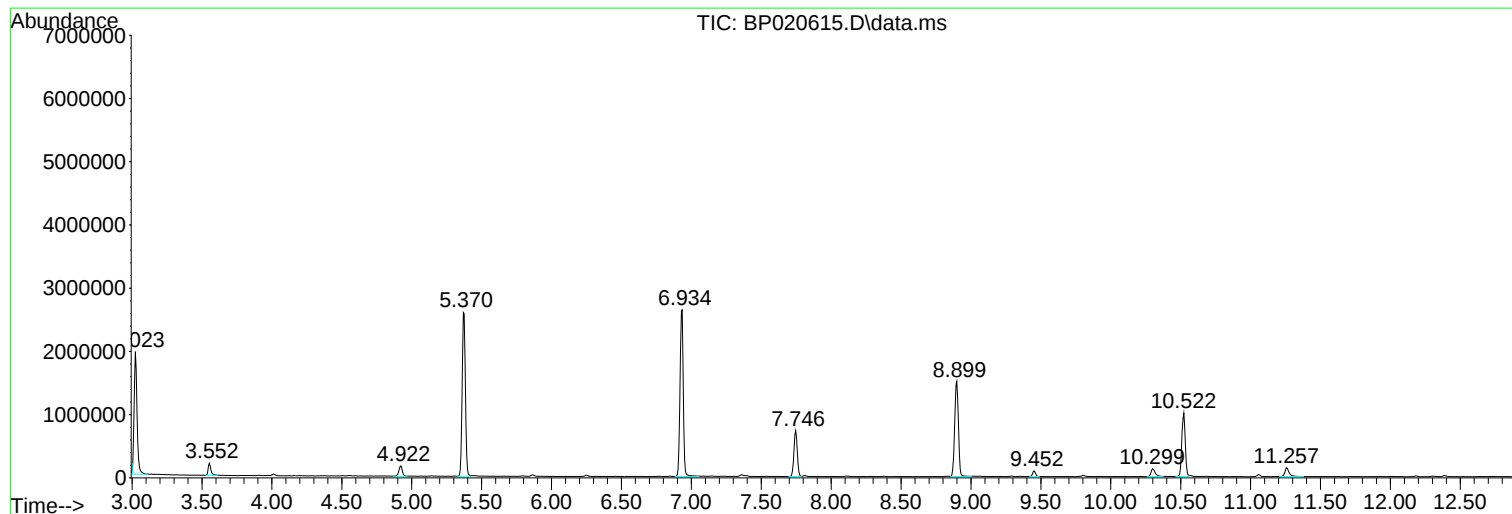
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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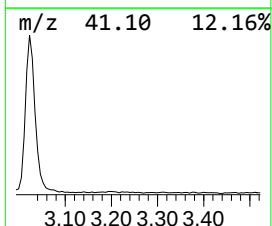
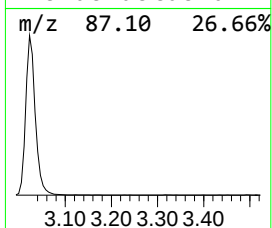
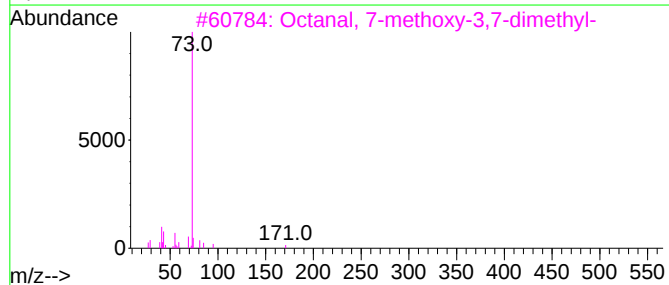
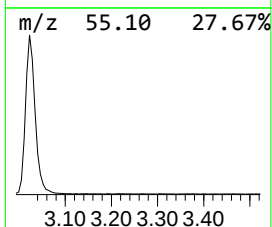
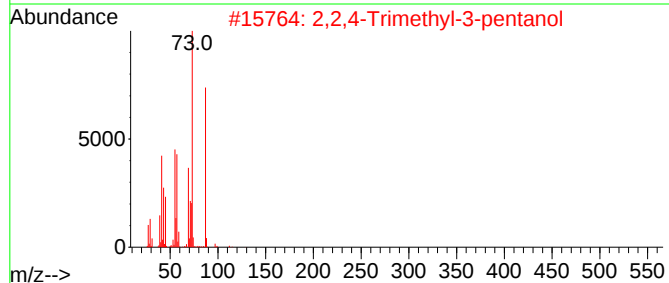
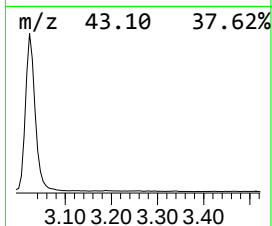
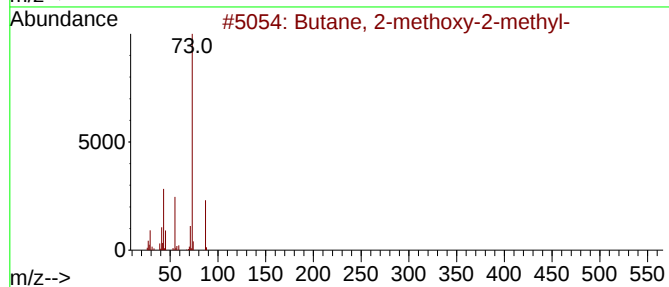
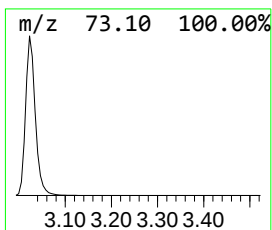
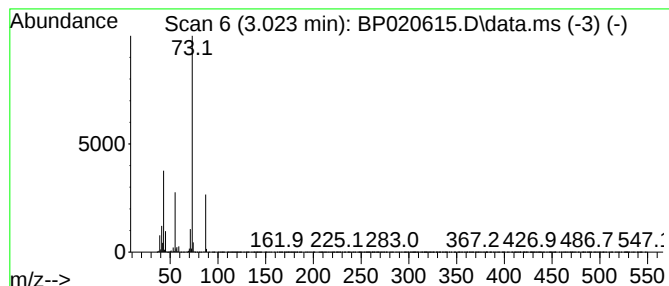
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.023	44.85 ng	2757620	1,4-Dichlorobenzene-d4	7.746

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			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	23
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17



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Misc :
ALS Vial : 7 Sample Multiplier: 1

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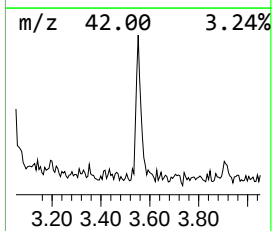
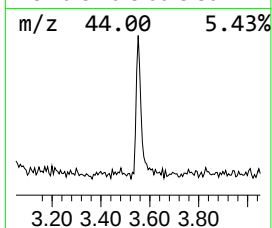
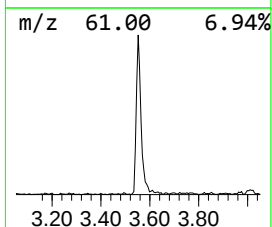
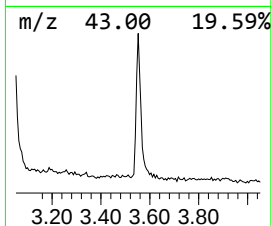
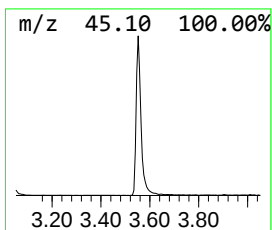
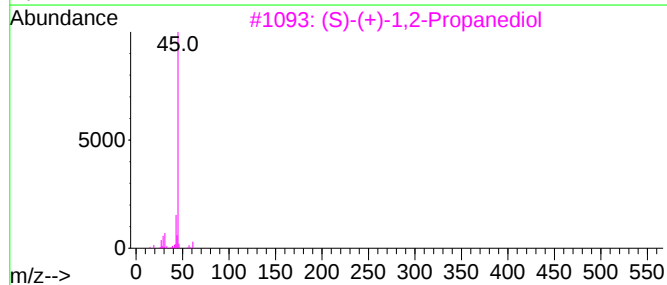
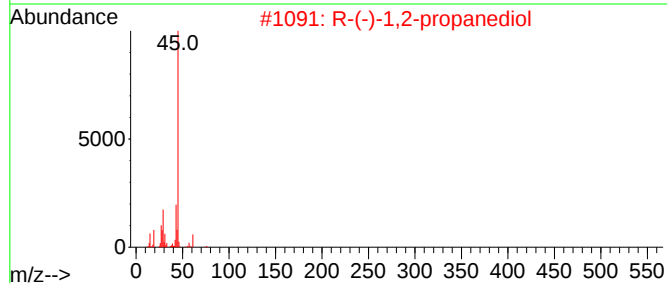
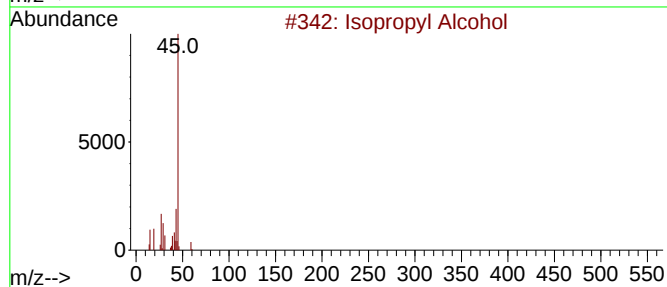
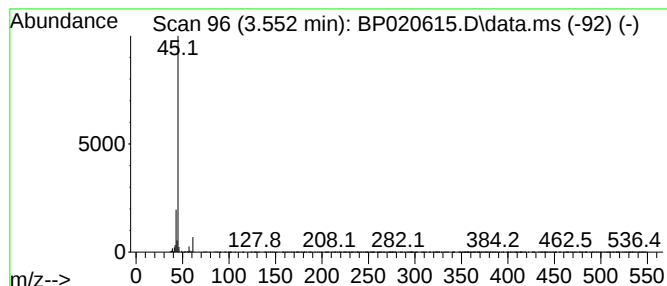
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Isopropyl Alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	4.25 ng	261219	1,4-Dichlorobenzene-d4	7.746

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	43
4		Propylene Glycol	76	C3H8O2	000057-55-6	38
5		Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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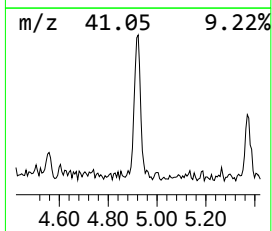
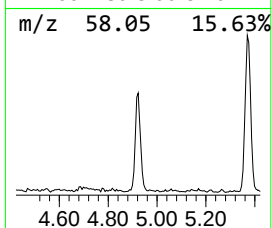
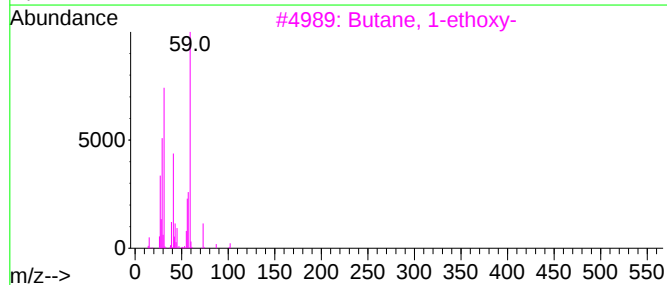
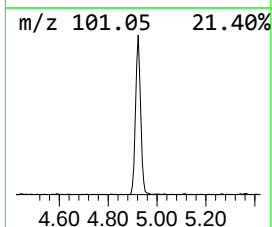
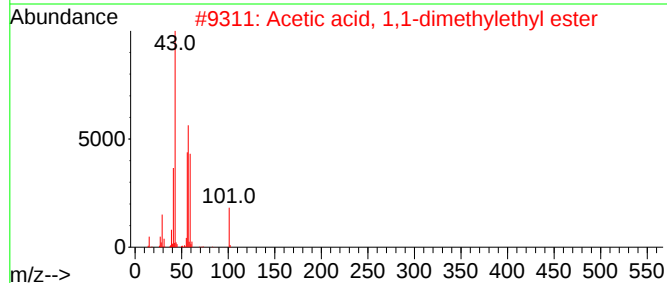
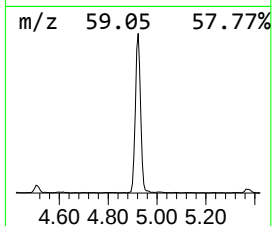
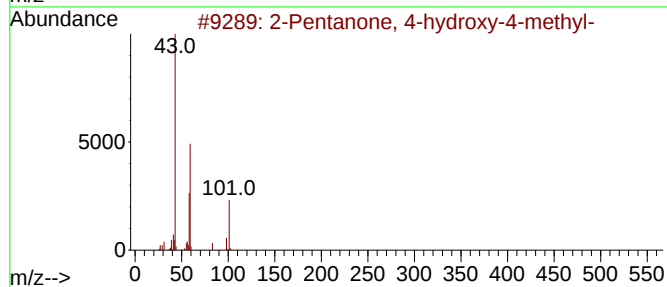
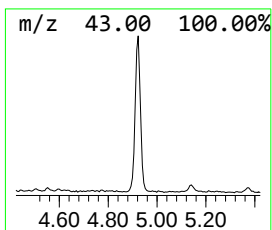
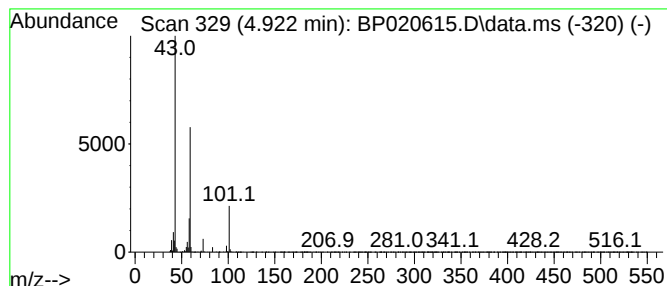
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	4.43 ng	272386	1,4-Dichlorobenzene-d4	7.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25
4			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23
5			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	17



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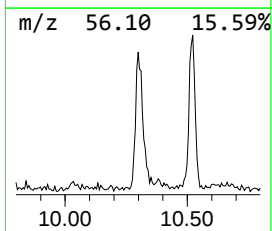
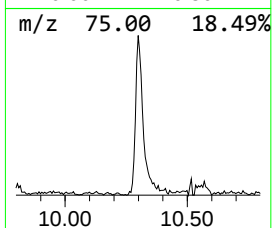
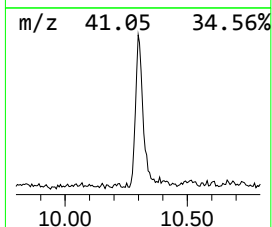
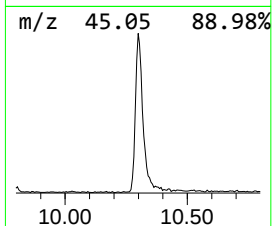
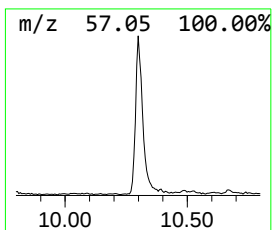
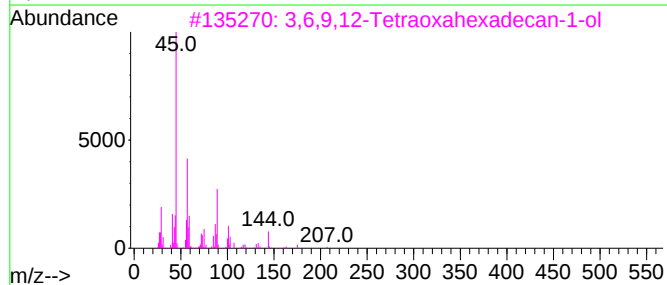
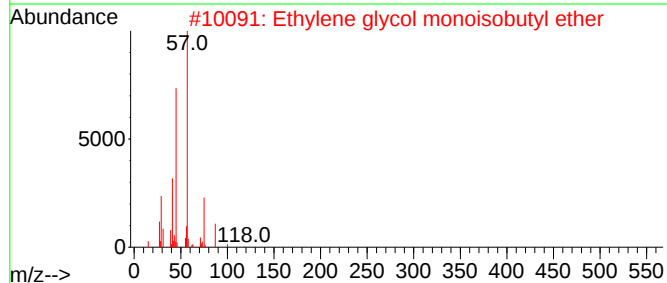
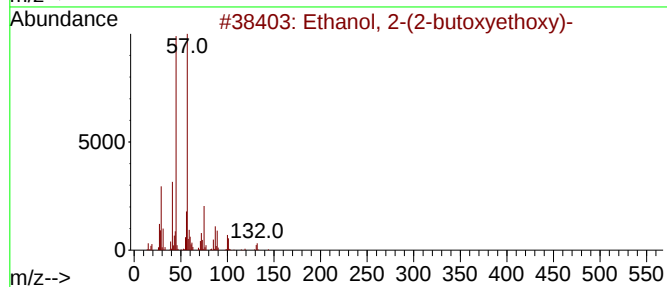
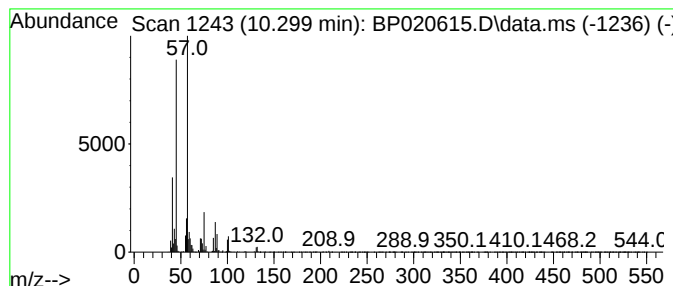
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.299	3.15 ng	267685	Naphthalene-d8	10.522	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2	Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
3	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	59
4	Ethanol, 2-[2-(2-methylpropoxy)e...	162	C8H18O3	018912-80-6	56
5	3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	53



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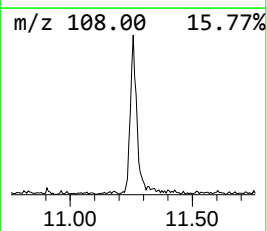
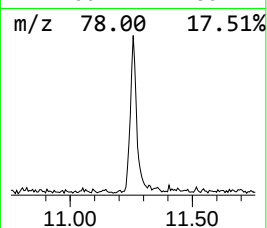
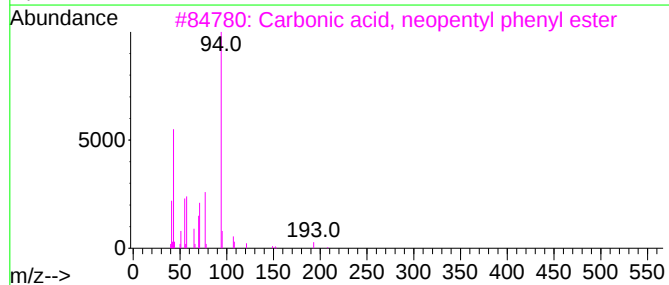
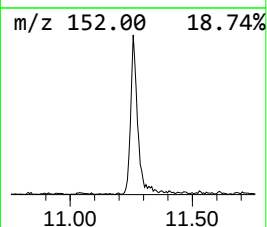
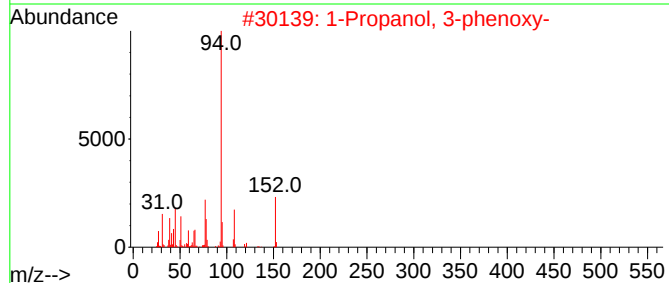
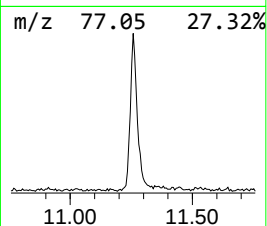
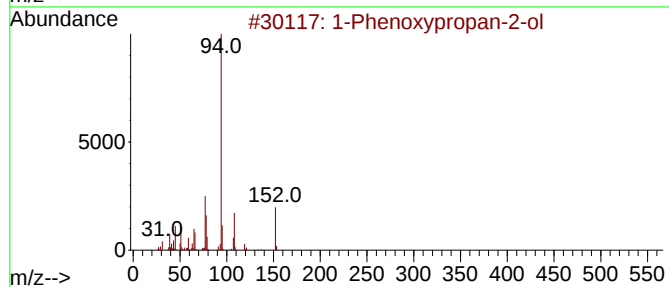
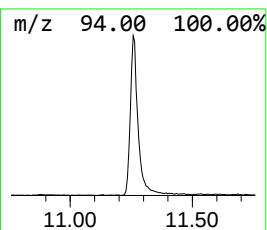
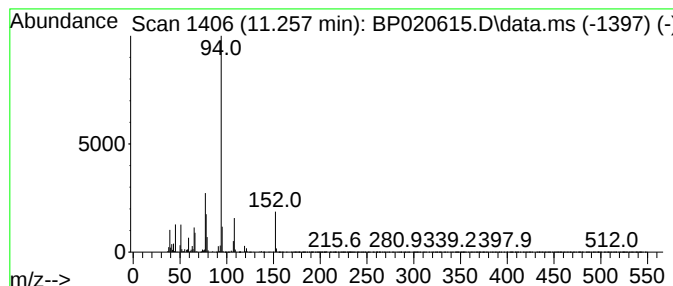
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.257	3.64 ng	309526	Naphthalene-d8	10.522

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2			1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	87
3			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
4			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5			2-Phenoxyethanol, isopropyl ether	180	C11H16O2	1000394-79-3	59



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020615.D
Acq On : 13 Jun 2024 17:22
Operator : MA/JU
Sample : P2855-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11989

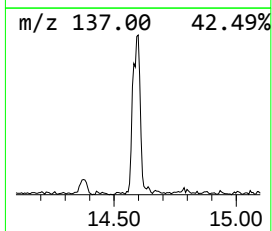
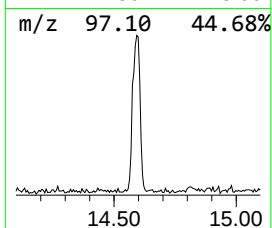
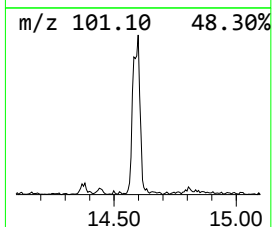
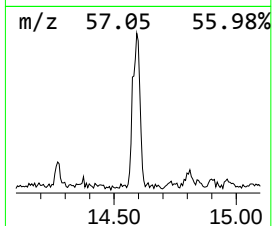
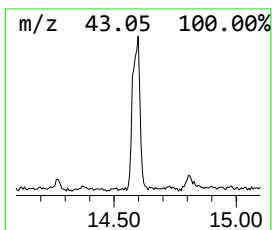
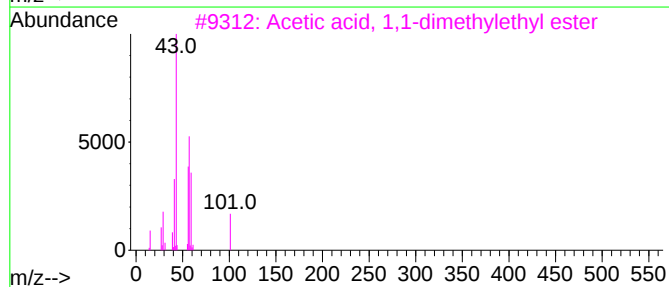
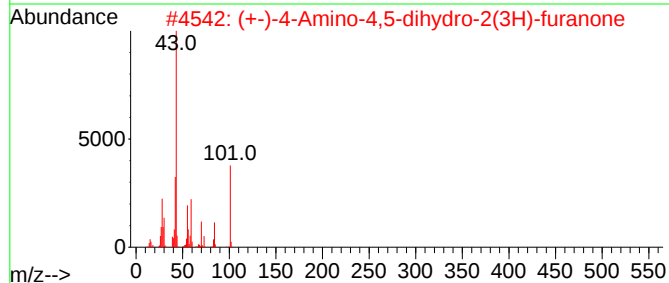
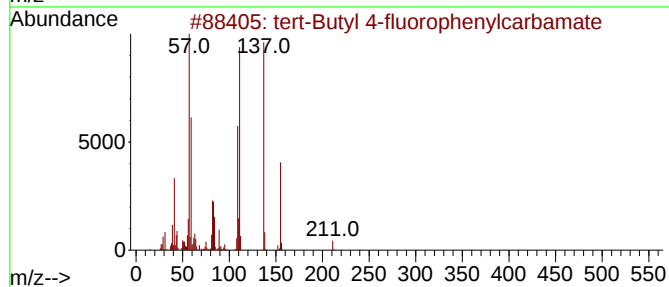
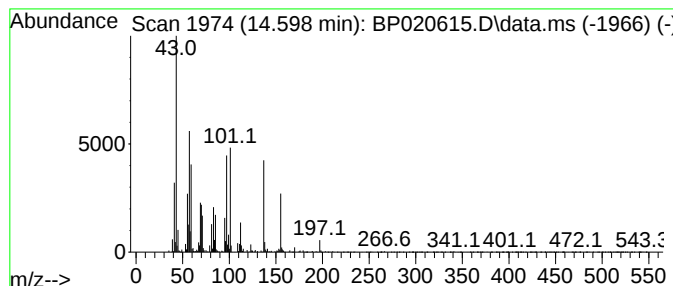
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.598 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.598	2.00 ng	228603	Acenaphthene-d10	14.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			tert-Butyl 4-fluorophenylcarbamate	211	C11H14FNO2	060144-53-8	16
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	16
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	14
4			Dodecane, 1-bromo-	248	C12H25Br	000143-15-7	11
5			Tetradecane, 1-bromo-	276	C14H29Br	000112-71-0	11



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020615.D
Acq On : 13 Jun 2024 17:22
Operator : MA/JU
Sample : P2855-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11989

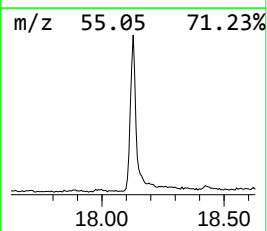
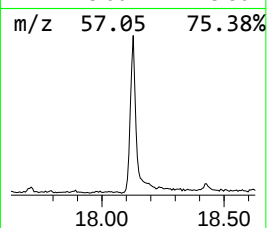
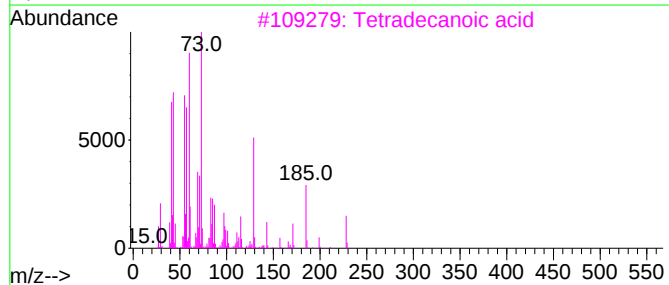
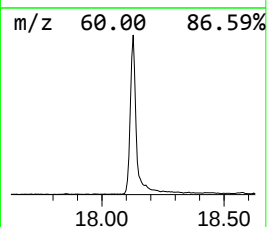
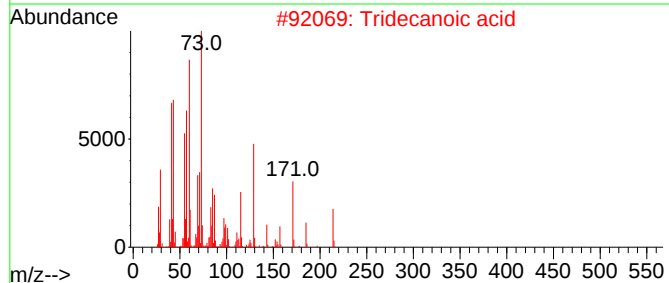
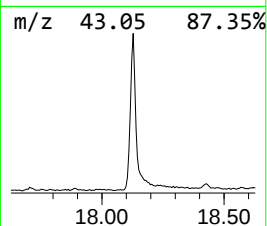
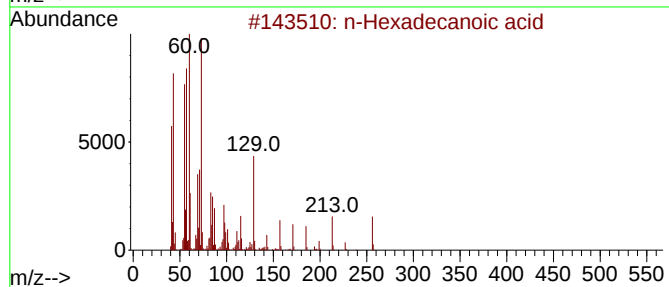
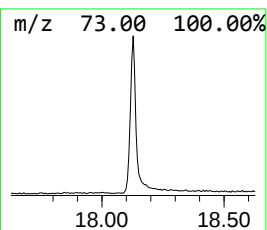
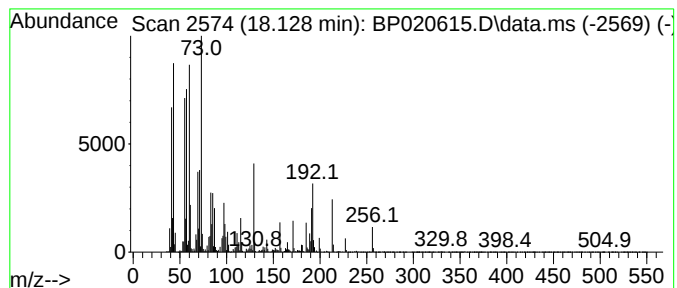
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.128	8.79 ng	1227230	Phenanthrene-d10	17.181

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	94
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	89
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
5			Octadecanoic acid	284	C18H36O2	000057-11-4	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020615.D
Acq On : 13 Jun 2024 17:22
Operator : MA/JU
Sample : P2855-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11989

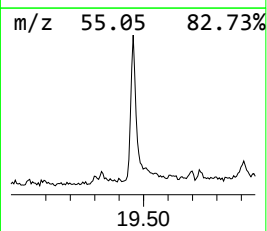
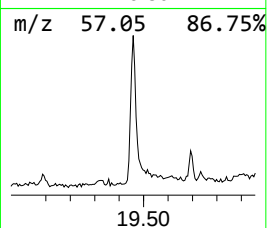
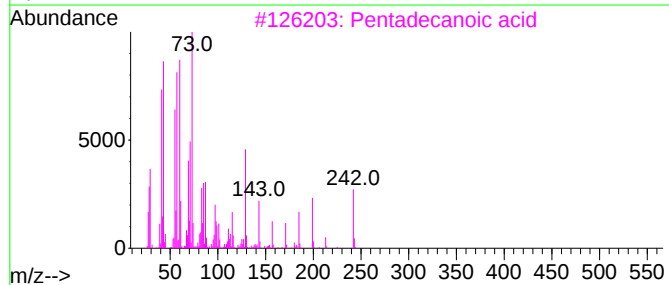
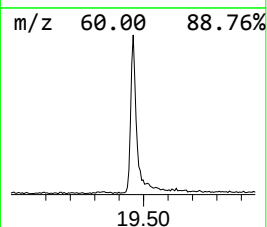
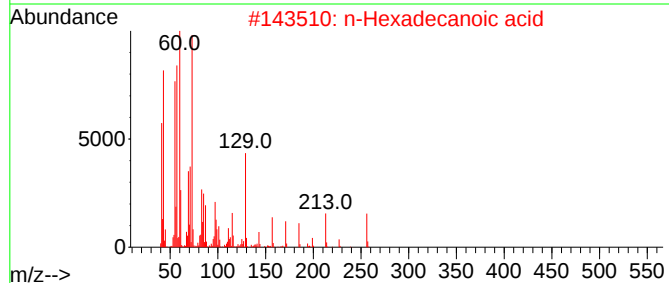
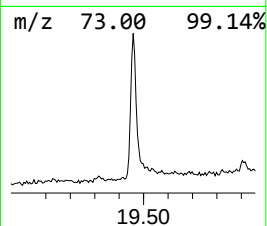
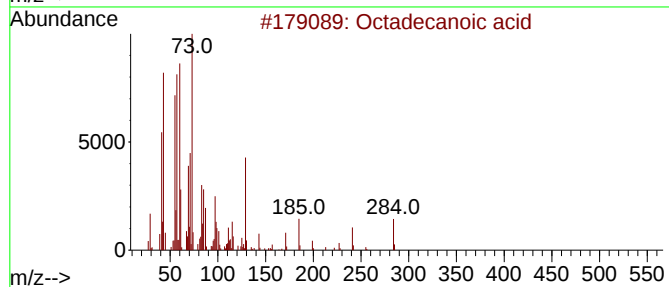
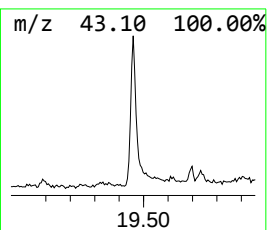
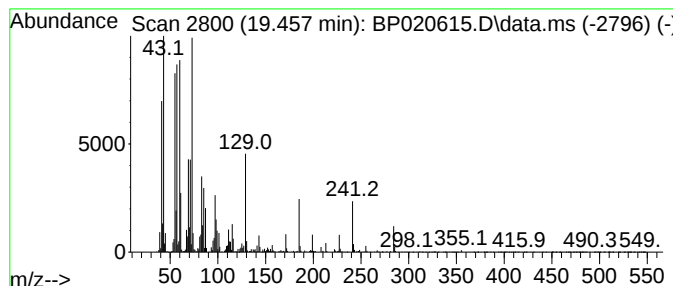
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	3.07 ng	550899	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	93
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
5			Tridecanoic acid	214	C13H26O2	000638-53-9	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020615.D
Acq On : 13 Jun 2024 17:22
Operator : MA/JU
Sample : P2855-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

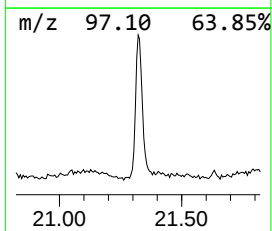
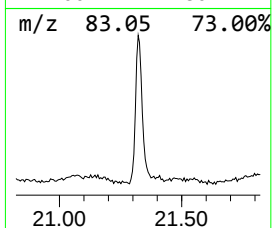
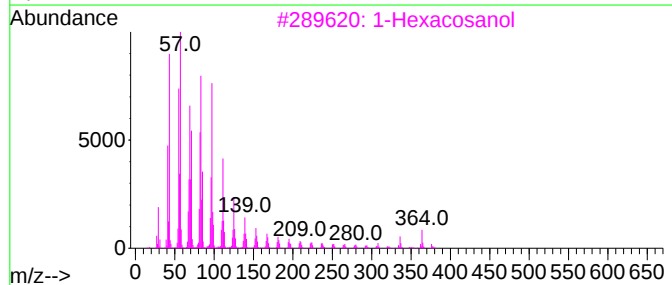
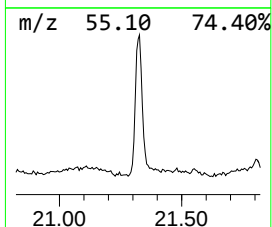
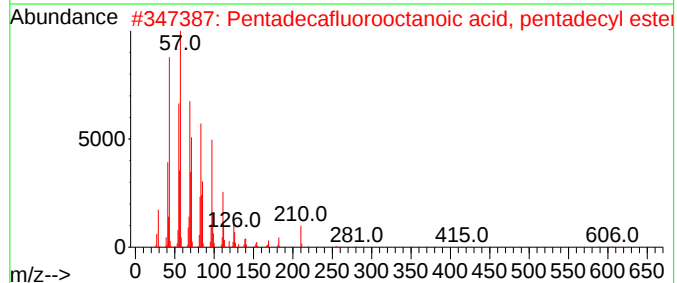
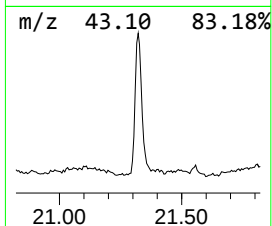
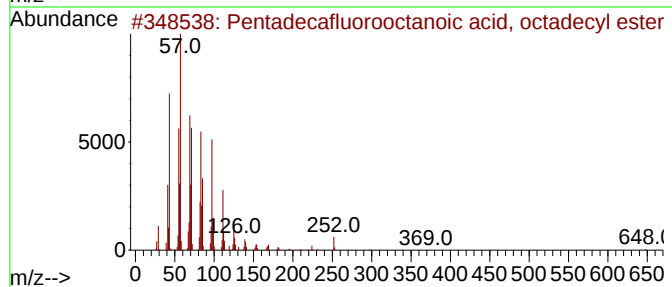
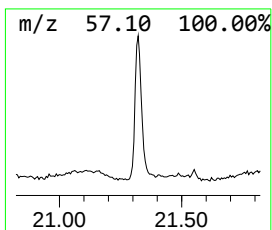
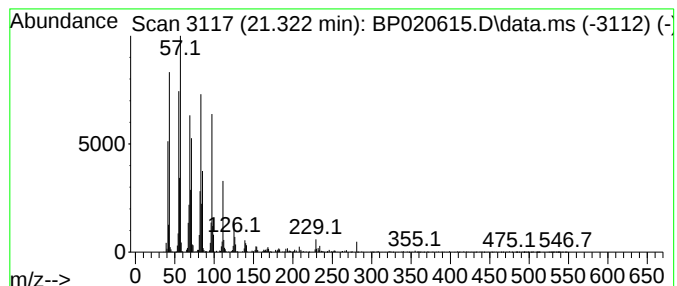
Instrument :
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
21.322	5.56 ng	998541	Chrysene-d12	21.633	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
2	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	93
3	1-Hexacosanol	382	C26H54O	000506-52-5	87
4	Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	87
5	Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	87



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061324\
Data File : BP020615.D
Acq On : 13 Jun 2024 17:22
Operator : MA/JU
Sample : P2855-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.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...	3.023	44.9	ng	2757620	1	7.746	1229740	20.0
Isopropyl Alcohol	3.552	4.3	ng	261219	1	7.746	1229740	20.0
2-Pentanone, 4-...	4.922	4.4	ng	272386	1	7.746	1229740	20.0
Ethanol, 2-(2-b...	10.299	3.1	ng	267685	2	10.522	1700130	20.0
1-Phenoxypropan...	11.257	3.6	ng	309526	2	10.522	1700130	20.0
unknown14.598	14.598	2.0	ng	228603	3	14.375	2285890	20.0
n-Hexadecanoic ...	18.128	8.8	ng	1227230	4	17.181	2791350	20.0
Octadecanoic acid	19.457	3.1	ng	550899	5	21.633	3591280	20.0
Pentadecafluoro...	21.322	5.6	ng	998541	5	21.633	3591280	20.0