

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
 Data File : BP020627.D
 Acq On : 14 Jun 2024 16:04
 Operator : MA/JU
 Sample : P2889-01
 Misc :
 ALS Vial : 6 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 WCS-TPJ

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: BP020627.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	19	rVB	2037448	2584945	20.23%	3.926%
2	3.552	93	96	108	rVB	188880	250167	1.96%	0.380%
3	4.922	322	329	336	rVB2	184810	295089	2.31%	0.448%
4	5.375	398	406	418	rBV	2938468	4558448	35.67%	6.923%
5	6.934	663	671	689	rBV	2899994	4673761	36.57%	7.098%
6	7.752	802	810	818	rBV	716019	1126406	8.81%	1.711%
7	8.899	998	1005	1020	rBV	1792370	3001273	23.49%	4.558%
8	10.522	1273	1281	1294	rBV	813089	1521687	11.91%	2.311%
9	11.263	1400	1407	1415	rBV2	89222	225937	1.77%	0.343%
10	12.993	1691	1701	1714	rBV	4694124	7718182	60.40%	11.722%
11	14.375	1927	1936	1944	rBV	1380120	2183528	17.09%	3.316%
12	14.610	1966	1976	1983	rBV	414322	1099487	8.60%	1.670%
13	15.892	2187	2194	2217	rBV	4071152	6612678	51.75%	10.043%
14	17.187	2407	2414	2419	rBV	1781425	2823904	22.10%	4.289%
15	17.228	2419	2421	2427	rVB	301282	358032	2.80%	0.544%
16	17.316	2432	2436	2441	rVB	124579	196060	1.53%	0.298%
17	18.122	2567	2573	2584	rBV	964858	1534142	12.01%	2.330%
18	18.292	2597	2602	2607	rBV3	78177	157938	1.24%	0.240%
19	19.316	2771	2776	2785	rBV	923130	1385091	10.84%	2.104%
20	19.457	2797	2800	2806	rBV	428806	572873	4.48%	0.870%
21	19.663	2831	2835	2836	rBV	142907	166638	1.30%	0.253%
22	19.692	2836	2840	2851	rVB	874797	1279642	10.01%	1.943%
23	19.916	2872	2878	2884	rBV	10391133	12778649	100.00%	19.407%
24	20.322	2944	2947	2950	rBV	112613	130062	1.02%	0.198%
25	20.651	2999	3003	3008	rBV	844390	1018922	7.97%	1.547%
26	21.322	3112	3117	3127	rVB4	517982	959820	7.51%	1.458%
27	21.633	3163	3170	3176	rBV2	1824963	3642351	28.50%	5.532%
28	24.974	3731	3738	3748	rBV	1132707	2988321	23.39%	4.538%

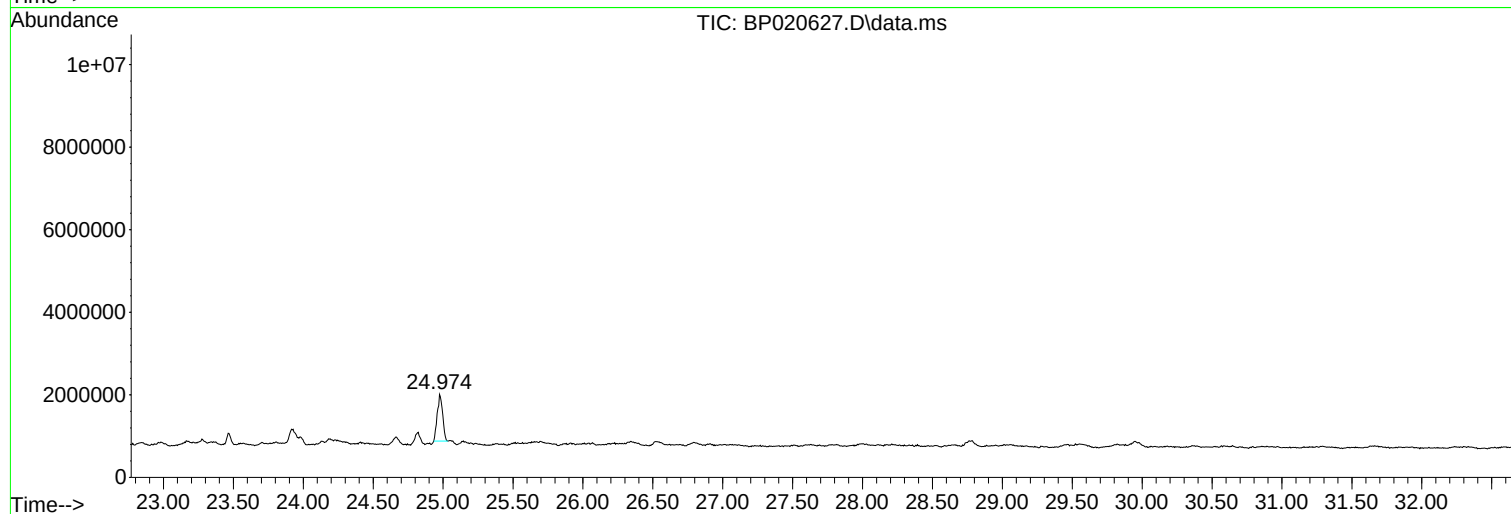
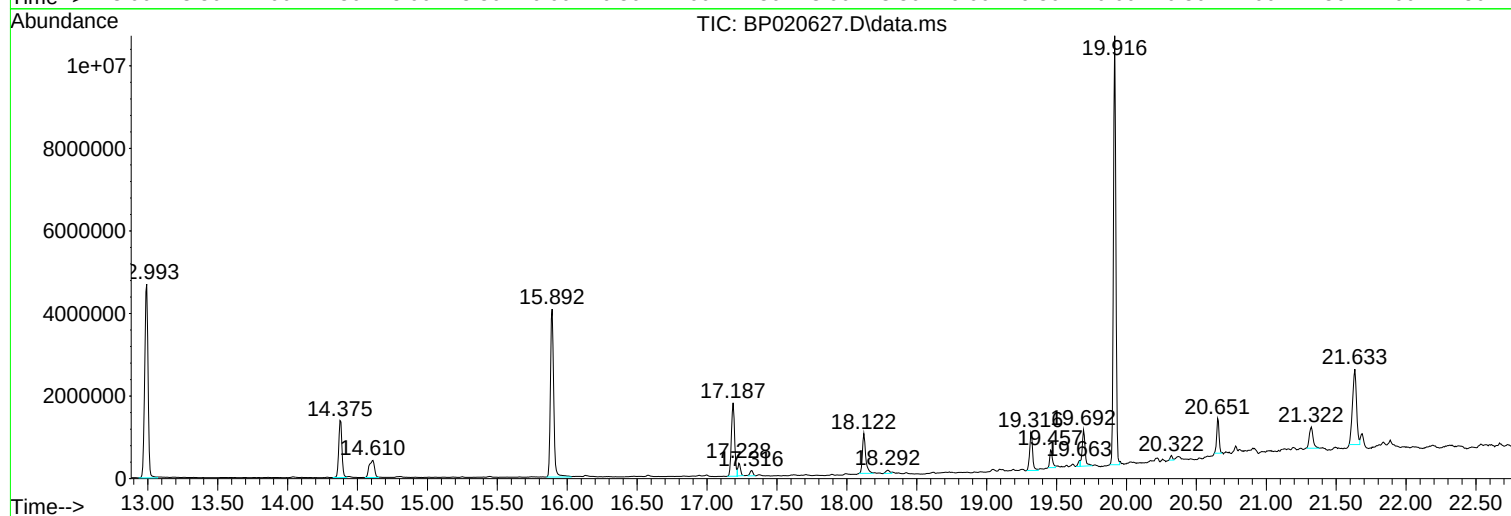
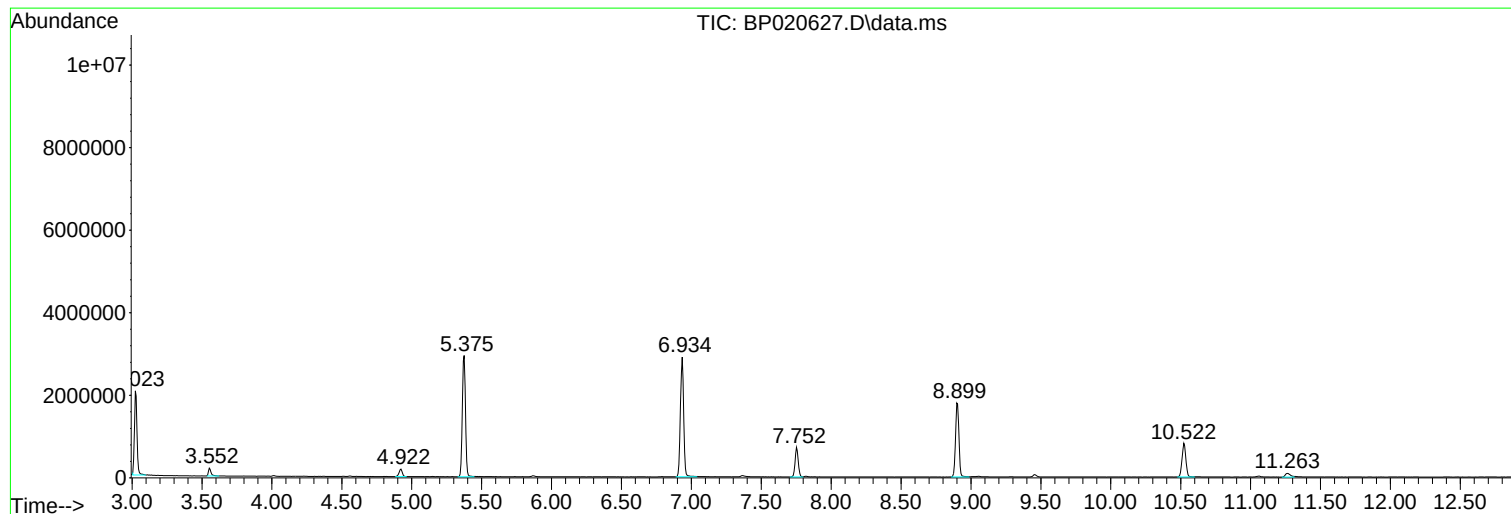
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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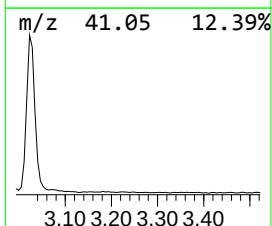
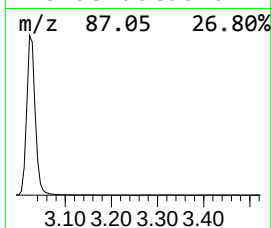
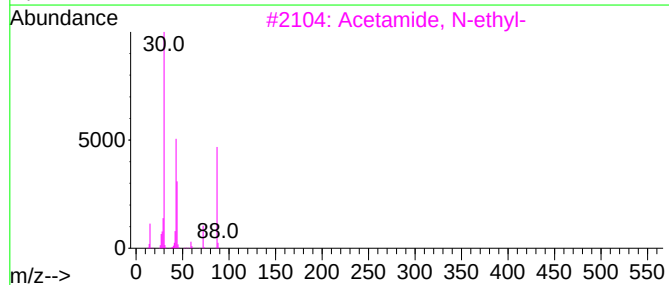
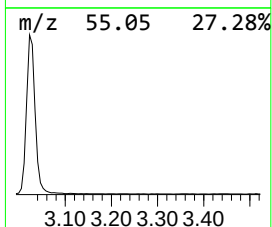
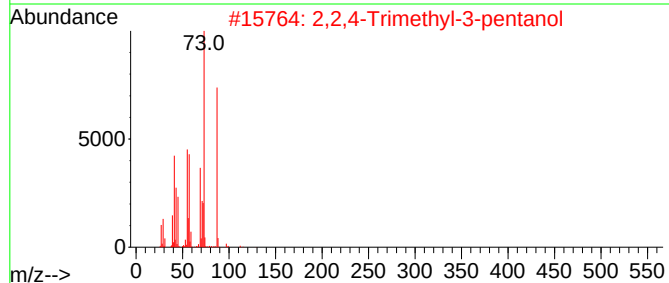
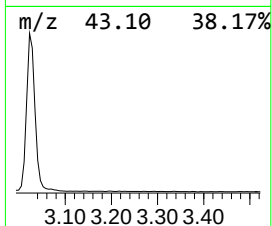
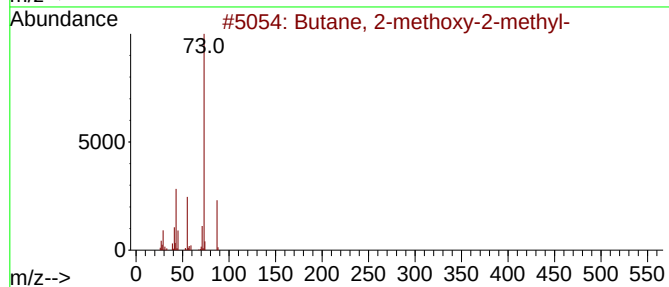
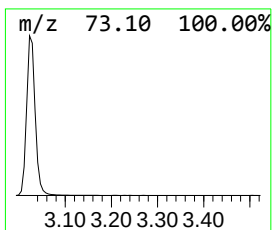
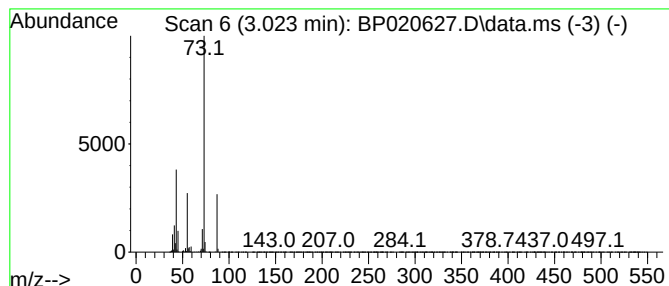
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	45.90 ng	2584950	1,4-Dichlorobenzene-d4	7.752

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
4			Octanal, 7-methoxy-3,7-dimethyl-	186	C11H22O2	003613-30-7	17
5			1,3-Dioxolane, 2-propyl-	116	C6H12O2	003390-13-4	17



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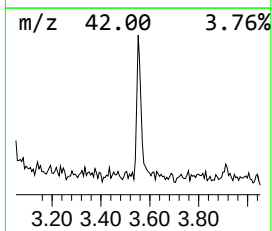
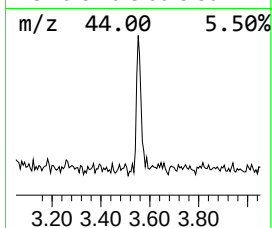
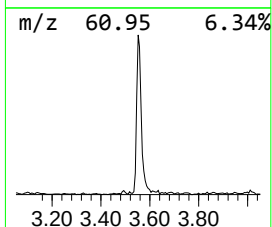
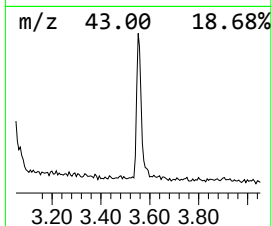
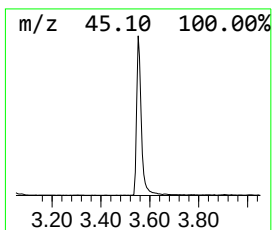
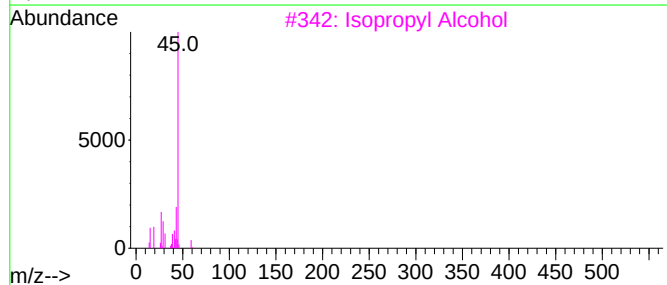
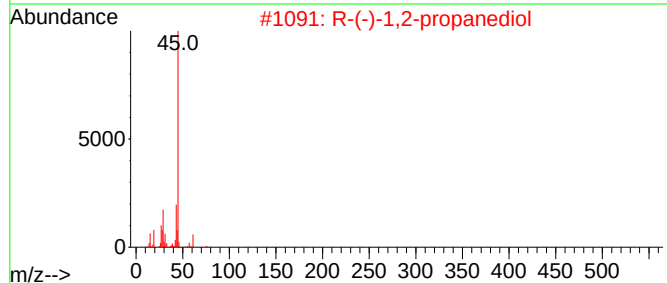
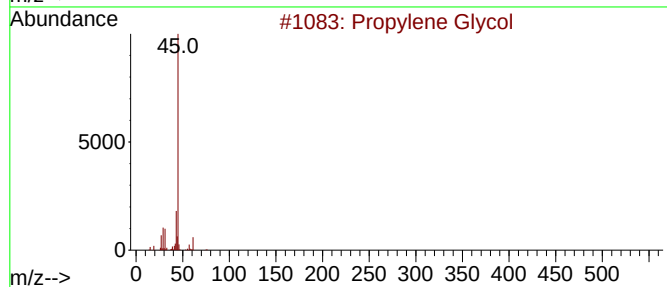
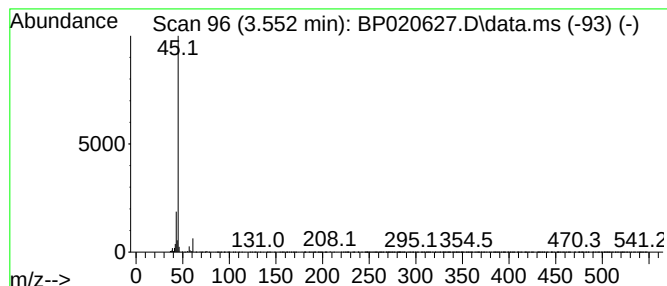
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	4.44 ng	250167	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	78
2			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9



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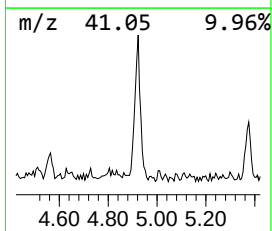
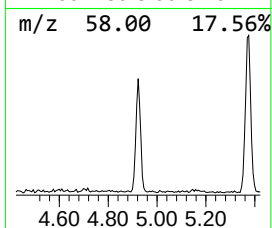
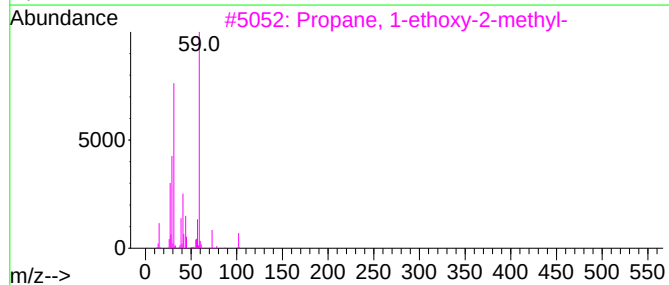
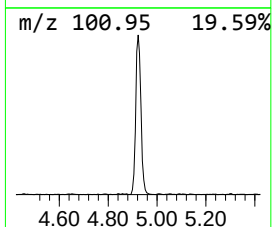
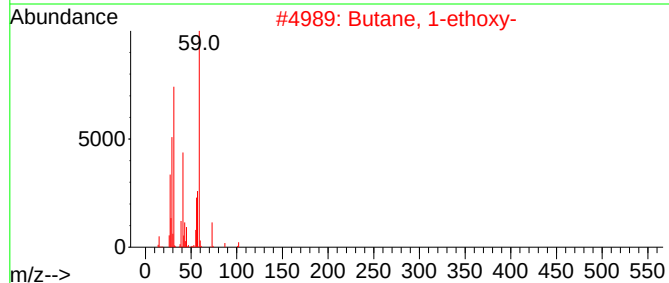
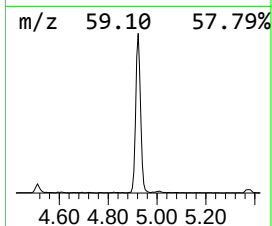
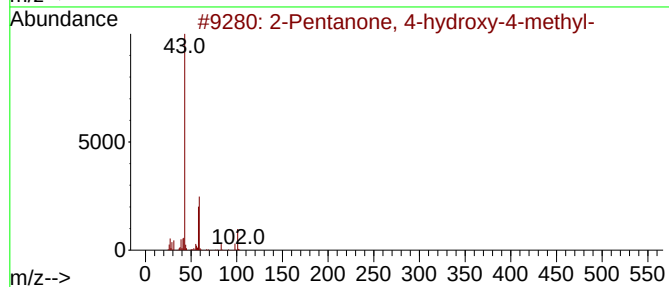
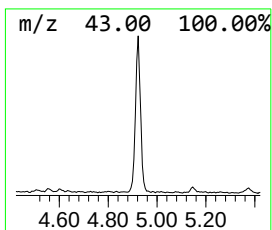
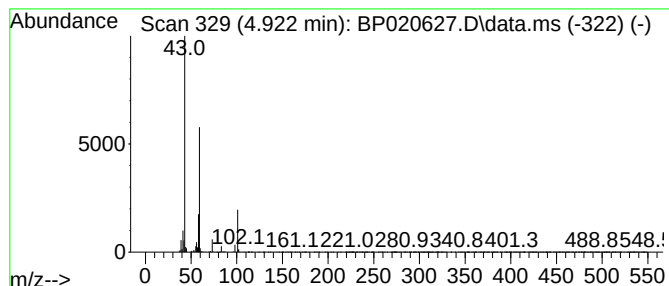
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.922	5.24 ng	295089	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25
3			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Acetone	58	C3H6O	000067-64-1	9



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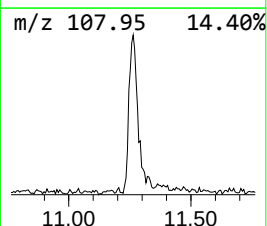
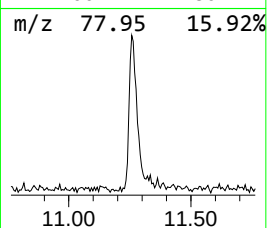
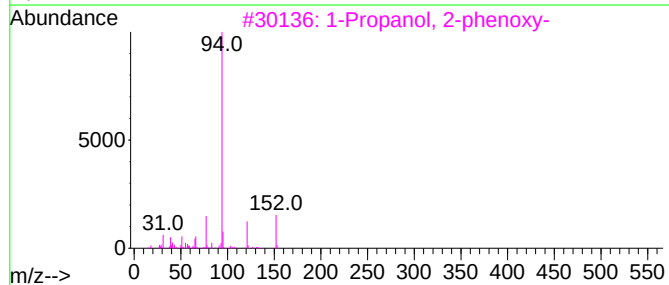
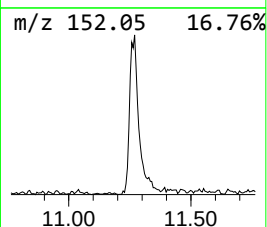
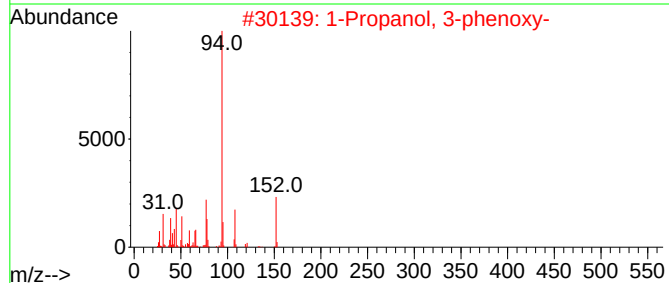
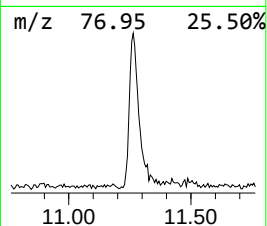
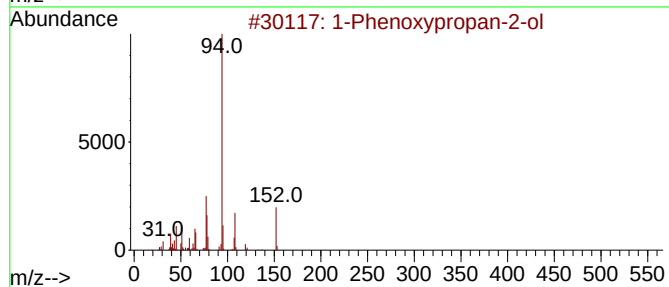
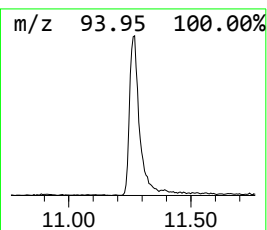
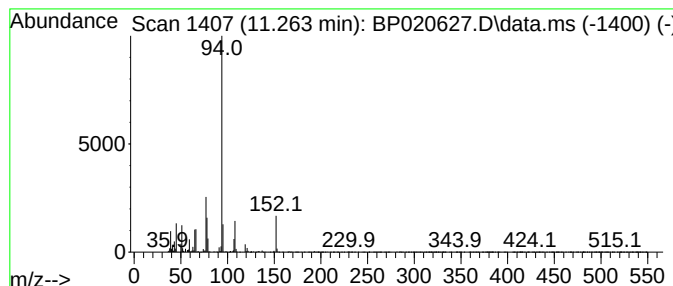
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	2.97 ng	225937	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	81
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	59
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59
5			3-Phenoxypropionic acid	166	C9H10O3	007170-38-9	53



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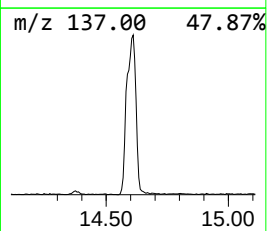
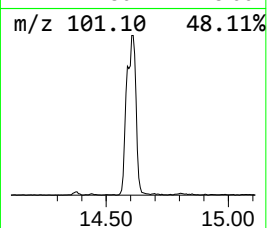
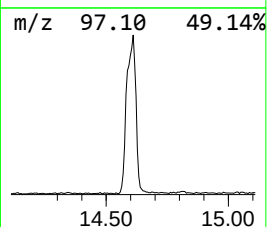
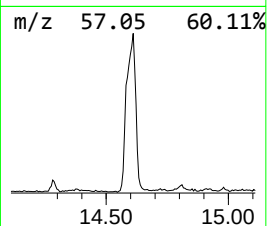
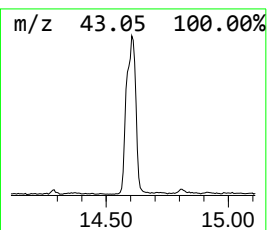
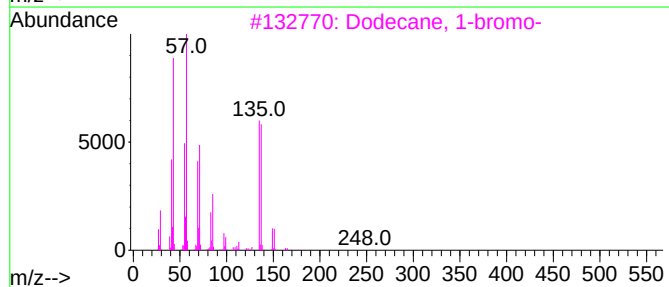
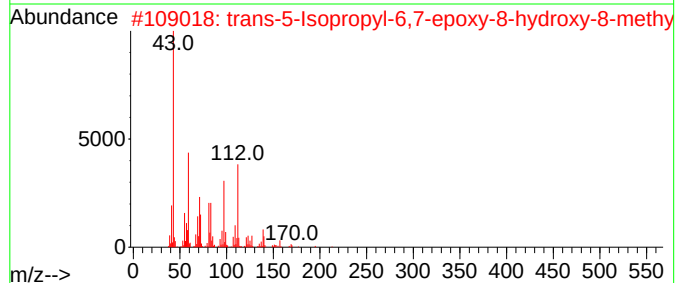
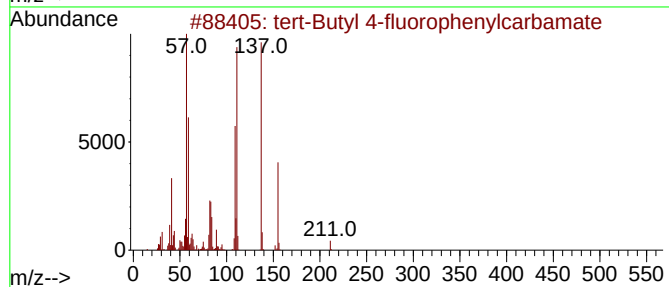
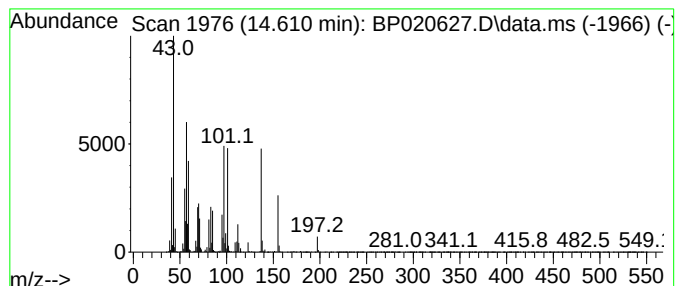
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.610 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.610	10.07 ng	1099490	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			trans-5-Isopropyl-6,7-epoxy-8-hy...	228	C13H24O3	058002-07-6	12
3			Dodecane, 1-bromo-	248	C12H25Br	000143-15-7	11
4			2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10



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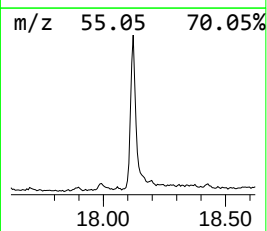
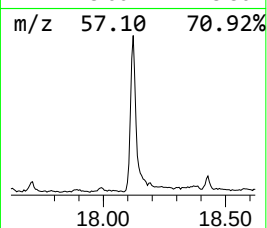
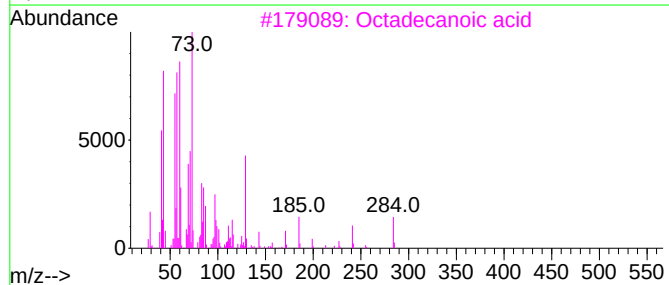
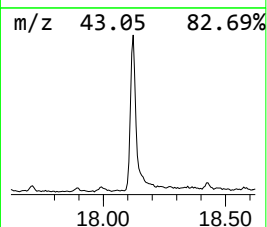
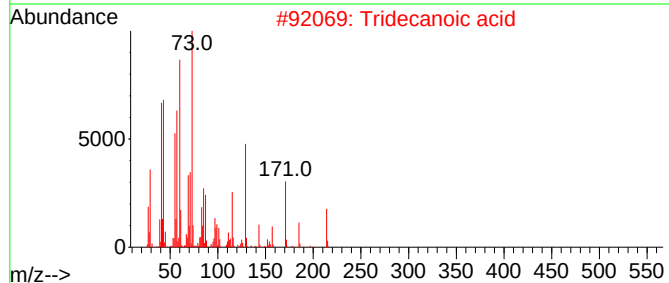
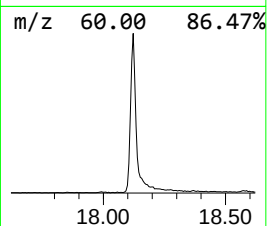
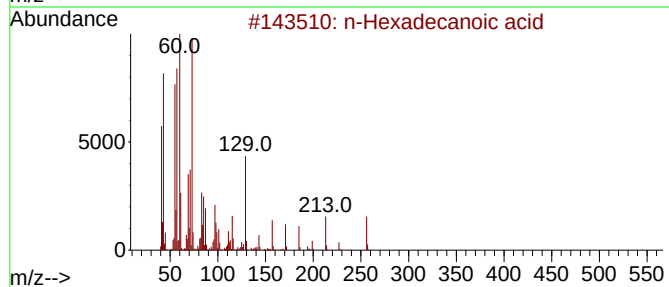
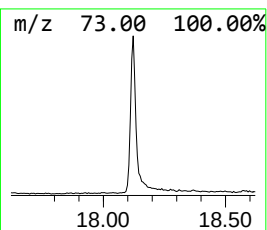
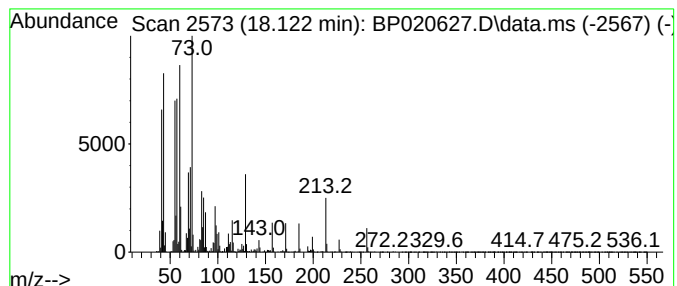
Instrument :
BNA_P
ClientSampleId :
WCS-TPJ

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 6 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD		R.T.	
18.122	10.87 ng	1534140	Phenanthrene-d10		17.186	
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	95
3	Octadecanoic acid		284	C18H36O2	000057-11-4	93
4	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
5	Tetradecanoic acid		228	C14H28O2	000544-63-8	89



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020627.D
Acq On : 14 Jun 2024 16:04
Operator : MA/JU
Sample : P2889-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPJ

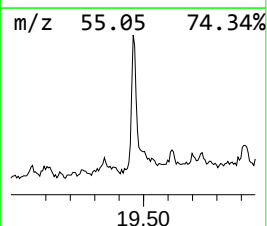
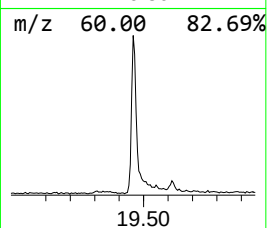
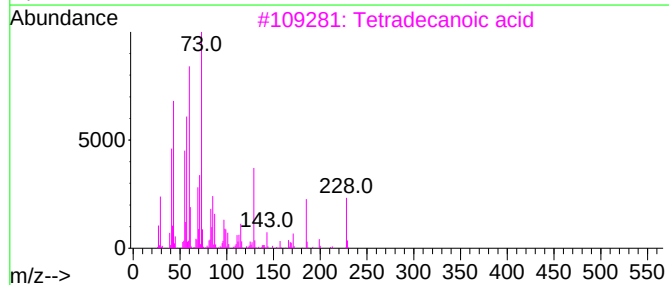
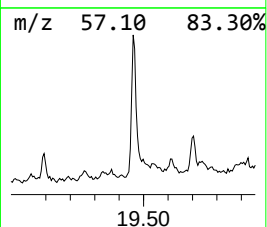
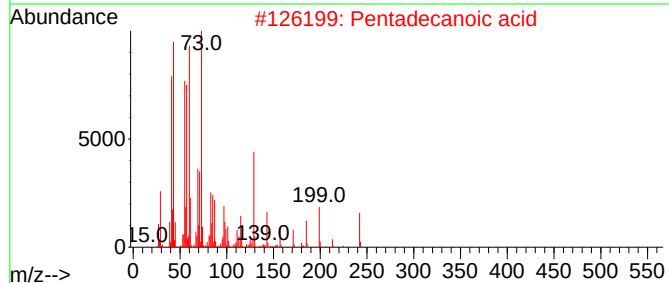
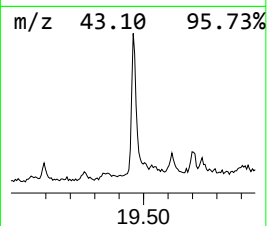
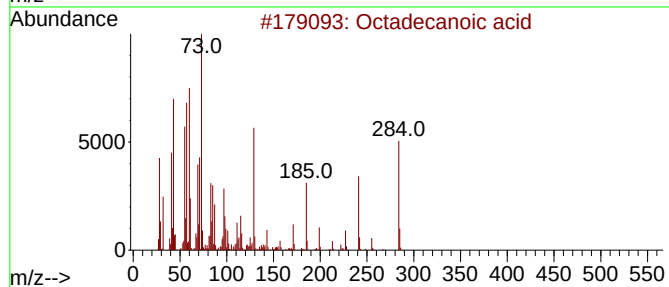
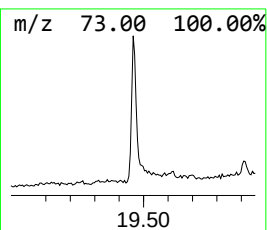
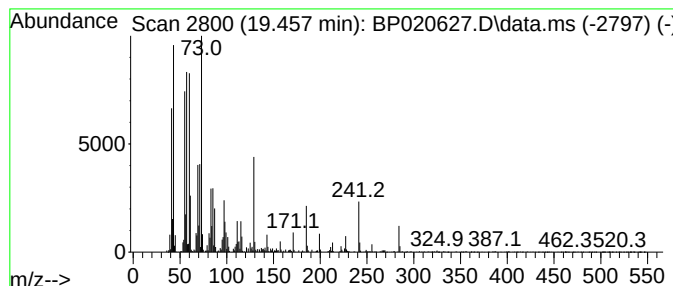
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.457	3.15 ng	572873	Chrysene-d12	21.633

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	91
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020627.D
Acq On : 14 Jun 2024 16:04
Operator : MA/JU
Sample : P2889-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPJ

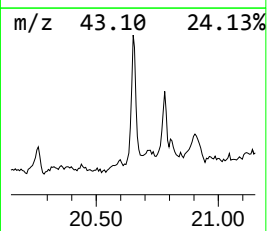
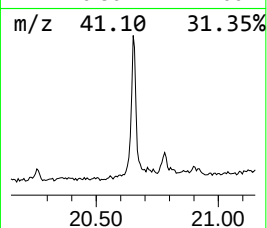
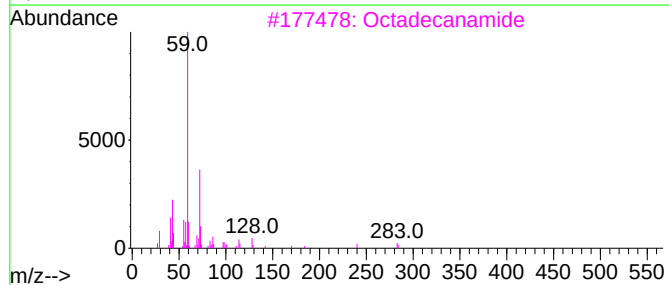
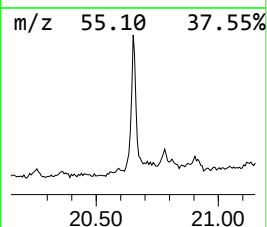
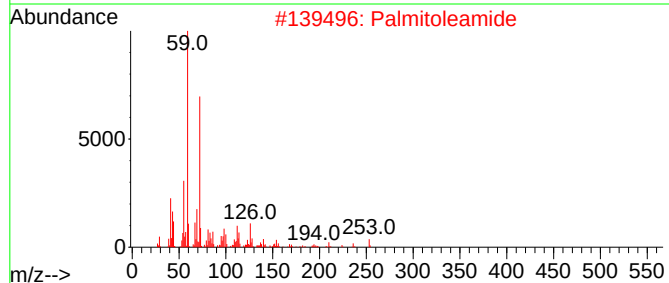
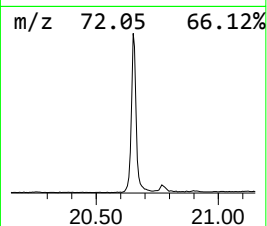
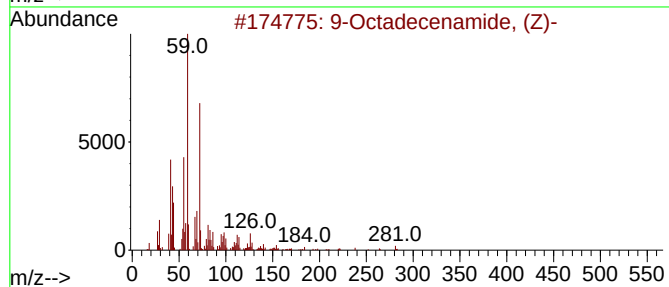
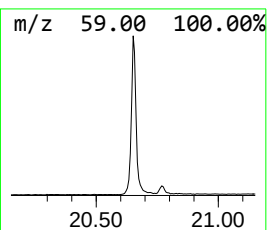
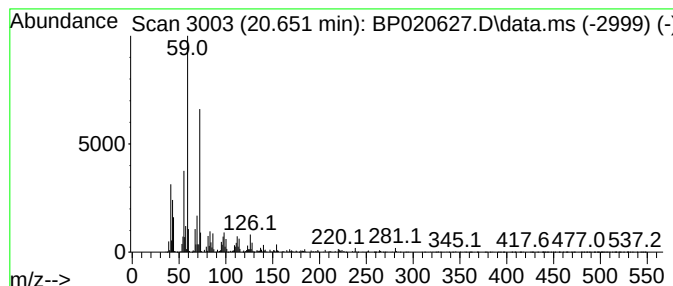
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 9-Octadecenamide, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.651	5.59 ng	1018920	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2			Palmitoleamide	253	C16H31NO	106010-22-4	91
3			Octadecanamide	283	C18H37NO	000124-26-5	59
4			Octanamide	143	C8H17NO	000629-01-6	59
5			Oxirane, tetramethyl-	100	C6H12O	005076-20-0	38



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020627.D
Acq On : 14 Jun 2024 16:04
Operator : MA/JU
Sample : P2889-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPJ

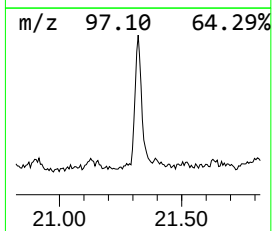
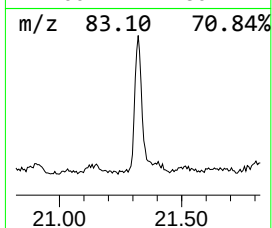
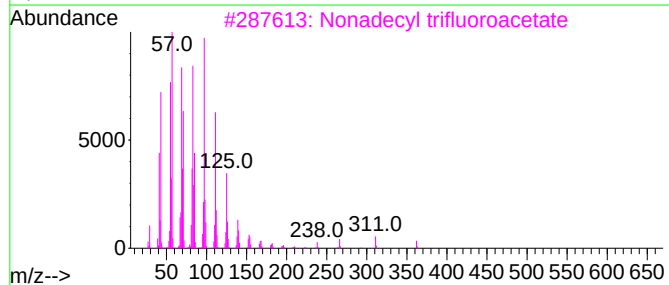
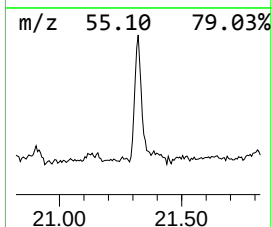
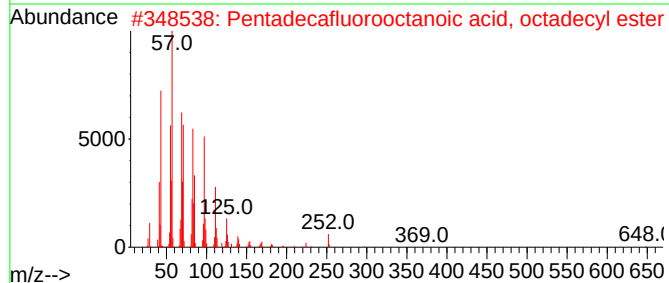
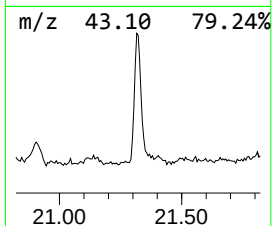
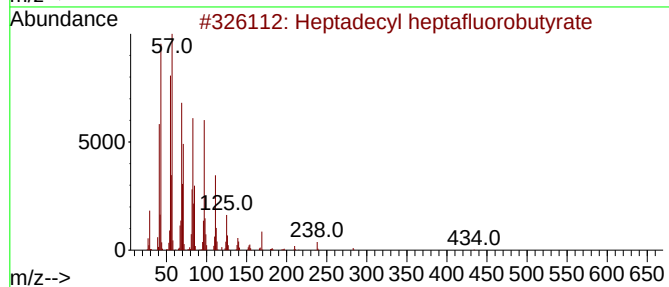
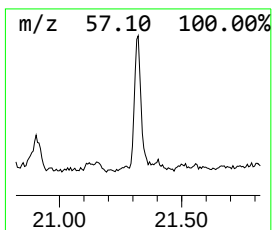
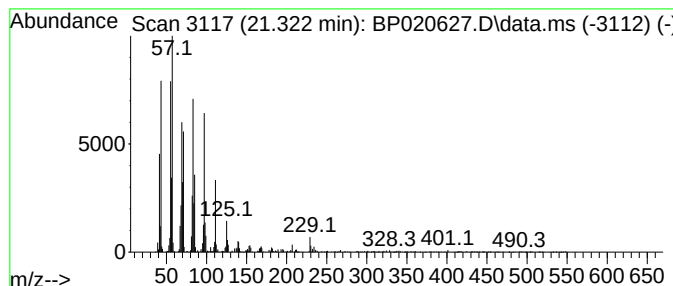
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Heptadecyl heptafluorobutyrate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.322	5.27 ng	959820	Chrysene-d12	21.633

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2			Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	94
3			Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	91
4			Pentafluoropropionic acid, octad...	416	C21H37F5O2	959261-25-7	91
5			Eicosyl trifluoroacetate	394	C22H41F3O2	1000351-75-2	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP061424\
Data File : BP020627.D
Acq On : 14 Jun 2024 16:04
Operator : MA/JU
Sample : P2889-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
WCS-TPJ

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	45.9	ng	2584950	1	7.752	1126410	20.0
Propylene Glycol	3.552	4.4	ng	250167	1	7.752	1126410	20.0
2-Pentanone, 4-...	4.922	5.2	ng	295089	1	7.752	1126410	20.0
1-Phenoxypropan...	11.263	3.0	ng	225937	2	10.522	1521690	20.0
unknown14.610	14.610	10.1	ng	1099490	3	14.375	2183530	20.0
n-Hexadecanoic ...	18.122	10.9	ng	1534140	4	17.186	2823900	20.0
Octadecanoic acid	19.457	3.1	ng	572873	5	21.633	3642350	20.0
9-Octadecenamid...	20.651	5.6	ng	1018920	5	21.633	3642350	20.0
Heptadecyl hept...	21.322	5.3	ng	959820	5	21.633	3642350	20.0