

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
 Data File : BP020562.D
 Acq On : 07 Jun 2024 16:14
 Operator : MA/JU
 Sample : P2707-05
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 SW-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-BP052924.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP020562.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.028	3	7	28	rVB	1887169	2906294	22.19%	3.745%
2	3.552	92	96	110	rBV	437586	601581	4.59%	0.775%
3	5.369	398	405	418	rBV	3659117	5697504	43.50%	7.342%
4	6.934	659	671	682	rBV	3804217	5829250	44.51%	7.512%
5	7.358	738	743	750	rBV	195470	316920	2.42%	0.408%
6	7.752	803	810	817	rBV	1361255	2050194	15.65%	2.642%
7	8.905	998	1006	1016	rBV	2180131	3837045	29.30%	4.945%
8	10.528	1272	1282	1289	rBV	1776471	2780192	21.23%	3.583%
9	11.263	1400	1407	1422	rBV	298927	534177	4.08%	0.688%
10	12.993	1694	1701	1717	rBV	5737137	8652987	66.07%	11.151%
11	14.387	1931	1938	1945	rBV	2512548	3658995	27.94%	4.715%
12	14.593	1968	1973	1975	rBV	778035	992045	7.57%	1.278%
13	15.792	2167	2177	2182	rBV2	80848	145052	1.11%	0.187%
14	15.904	2189	2196	2204	rBV	4774167	7019246	53.60%	9.046%
15	17.192	2409	2415	2420	rBV	3131034	4325840	33.03%	5.575%
16	17.910	2533	2537	2542	rVB	121921	161781	1.24%	0.208%
17	18.151	2573	2578	2585	rBV	980075	1333859	10.18%	1.719%
18	19.139	2742	2746	2753	rVB	247181	355413	2.71%	0.458%
19	19.333	2774	2779	2791	rVV	303817	600079	4.58%	0.773%
20	19.480	2799	2804	2817	rBV2	288221	532517	4.07%	0.686%
21	19.710	2840	2843	2855	rVB	225774	395728	3.02%	0.510%
22	19.939	2874	2882	2892	rVB	8209747	13096728	100.00%	16.878%
23	21.345	3116	3121	3128	rVB	799183	1224115	9.35%	1.578%
24	21.663	3168	3175	3181	rBV2	2819336	5009361	38.25%	6.456%
25	23.527	3487	3492	3500	rVB2	196214	419826	3.21%	0.541%
26	25.021	3737	3746	3758	rVB2	1874210	5119800	39.09%	6.598%

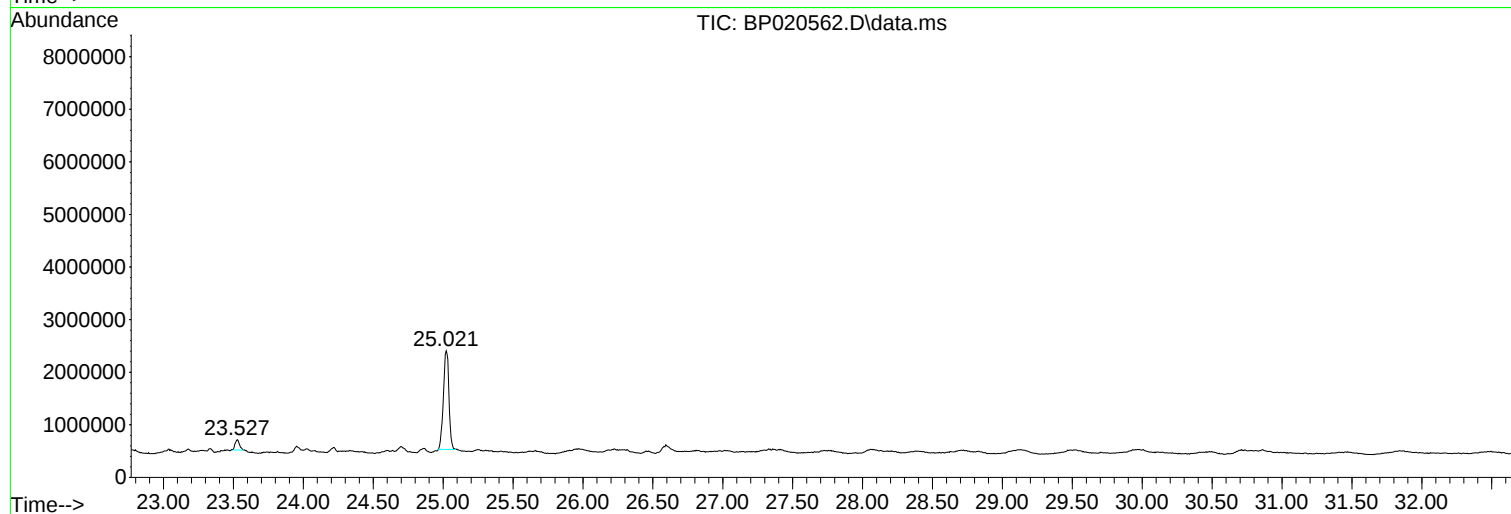
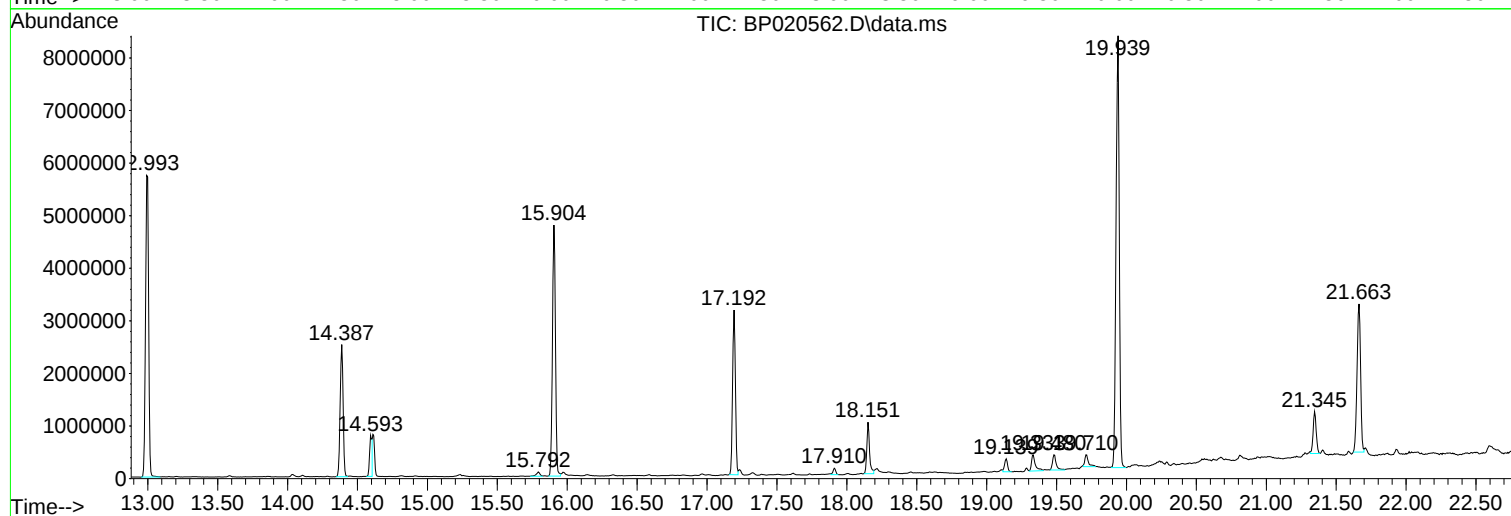
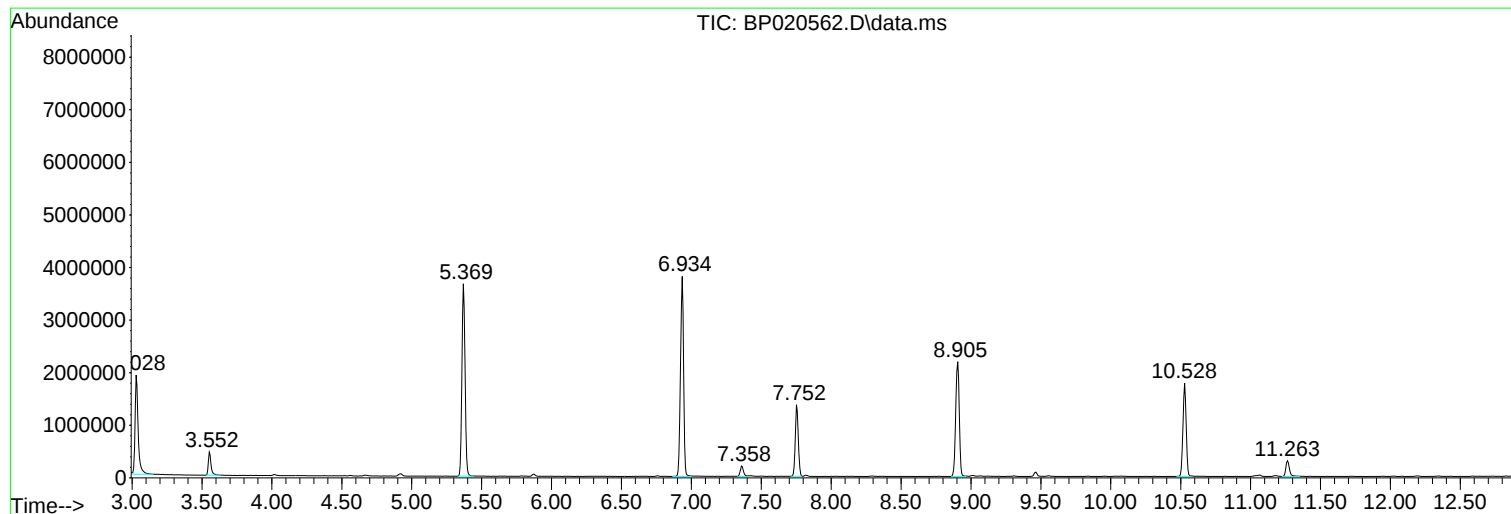
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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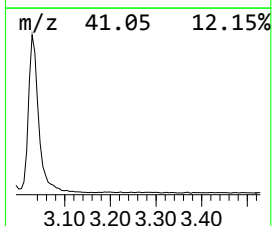
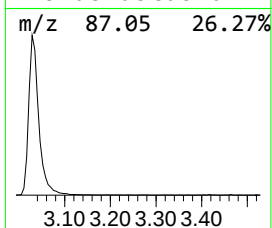
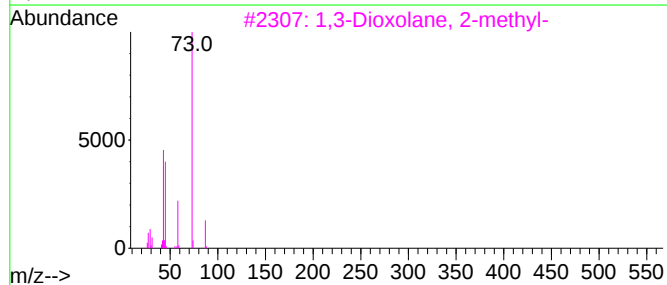
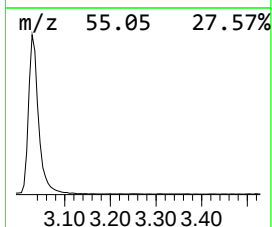
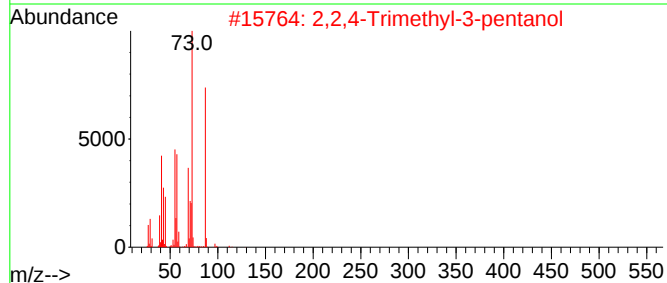
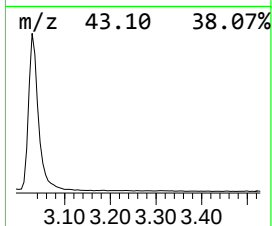
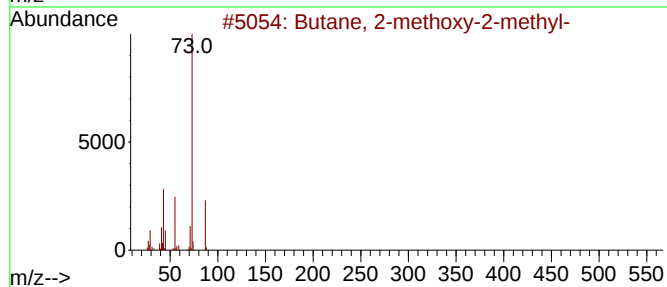
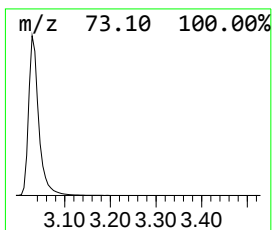
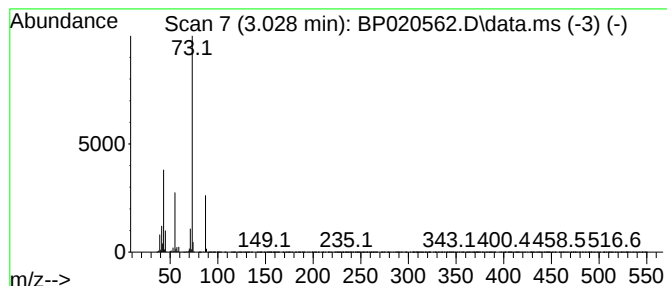
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.028	28.35 ng	2906290	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	39
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	37
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12
5			Borane, dimethoxy-	74	C2H7BO2	004542-61-4	9



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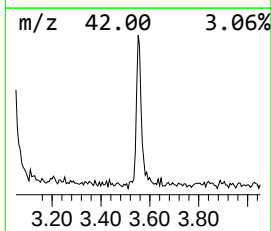
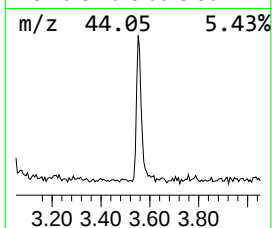
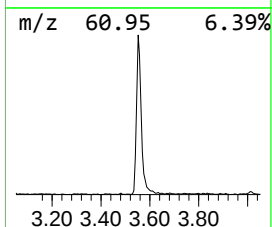
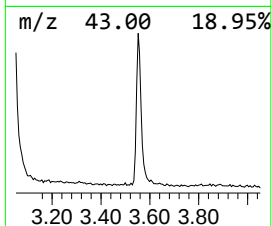
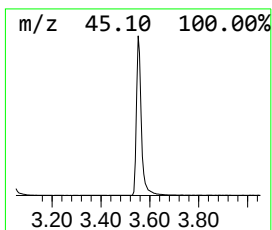
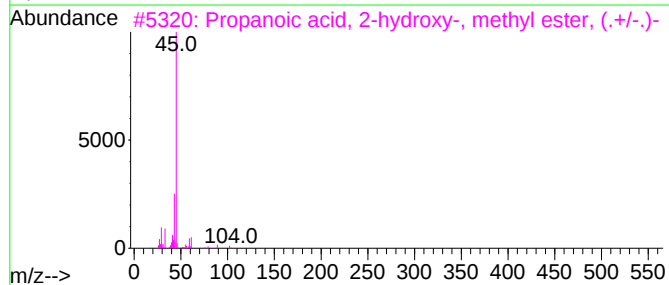
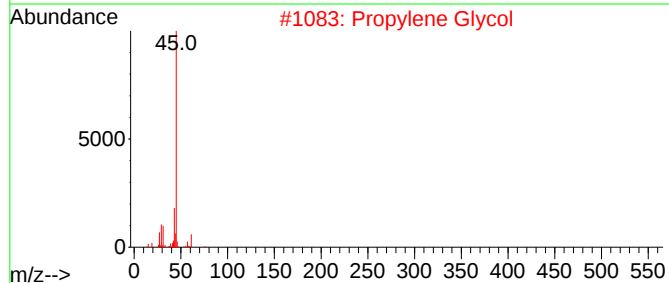
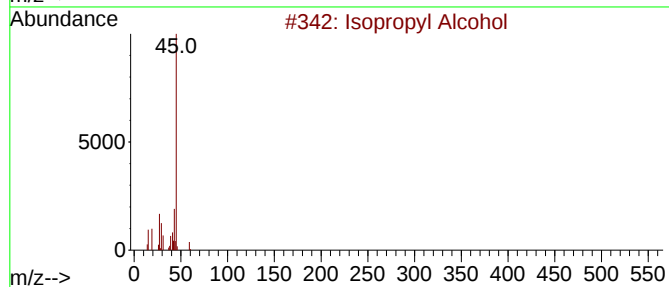
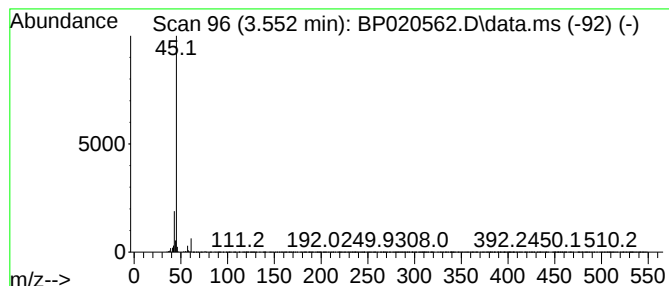
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.552	5.87 ng	601581	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
2			Propylene Glycol	76	C3H8O2	000057-55-6	47
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9
5			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9



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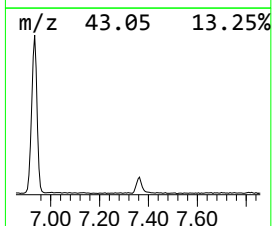
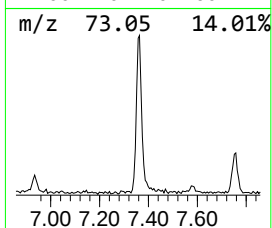
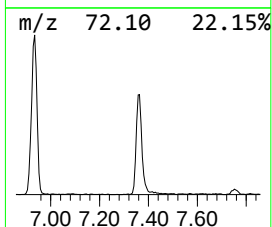
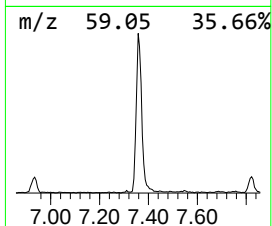
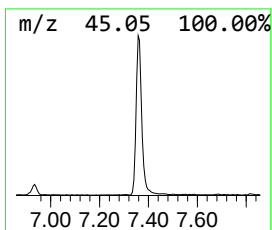
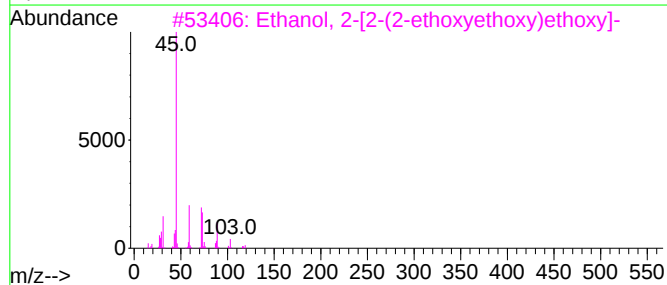
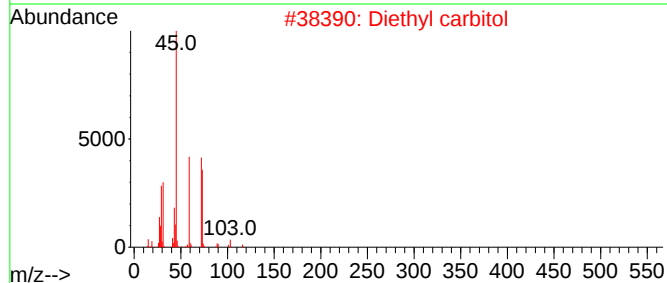
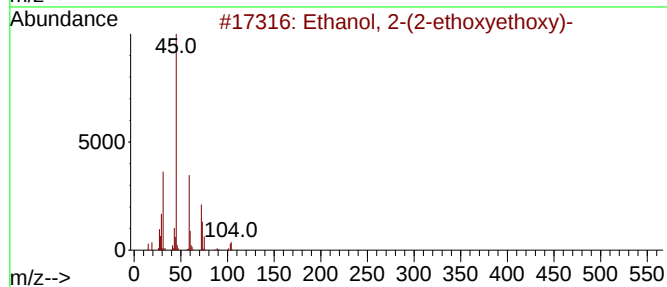
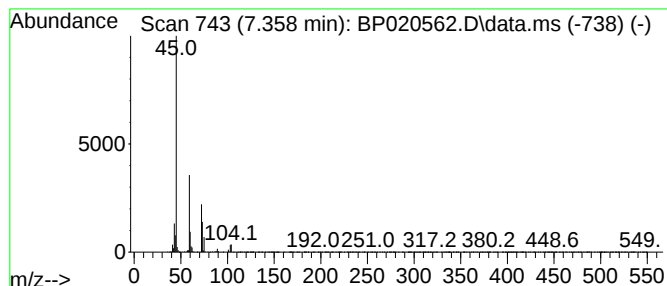
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-(2-ethoxyethoxy)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.358	3.09 ng	316920	1,4-Dichlorobenzene-d4	7.752

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-ethoxyethoxy)-	134	C6H14O3	000111-90-0	90
2			Diethyl carbitol	162	C8H18O3	000112-36-7	72
3			Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	50
4			2-Butanol, 3-methyl-	88	C5H12O	000598-75-4	47
5			2-Propanol, 1-(1-methylethoxy)-	118	C6H14O2	003944-36-3	45



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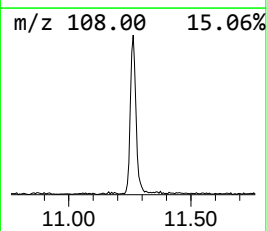
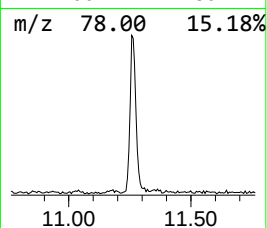
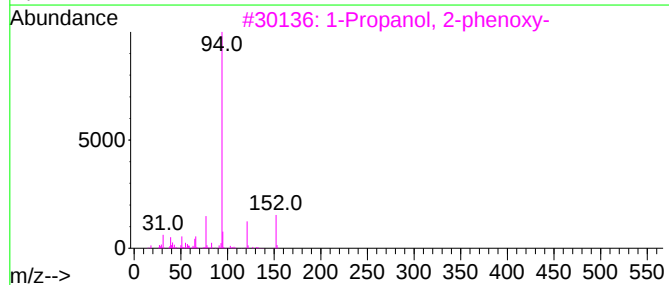
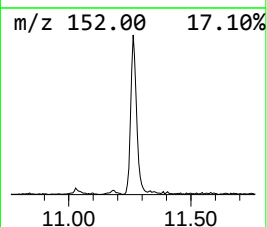
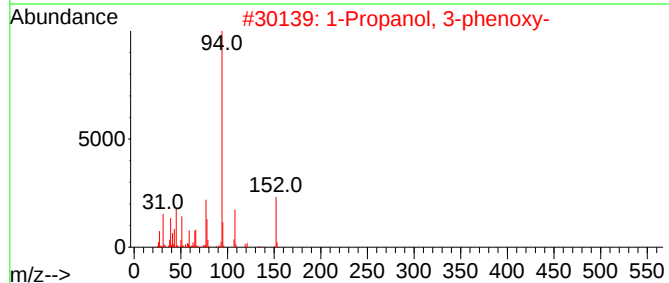
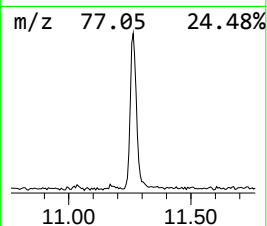
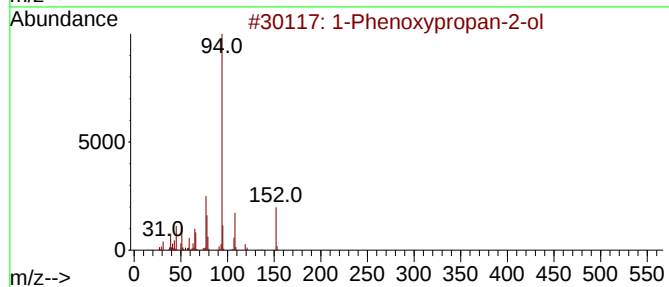
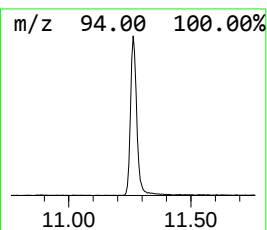
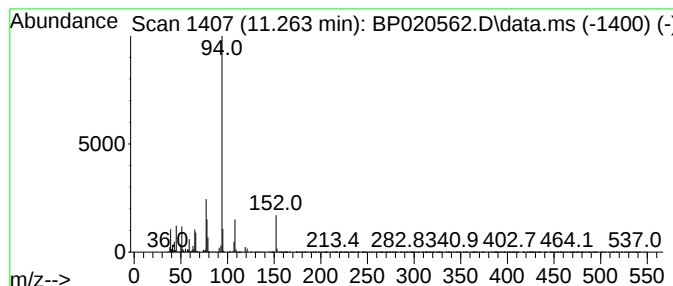
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Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.263	3.84 ng	534177	Naphthalene-d8	10.528

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	93
3			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4			Carbonic acid, sec-butyl phenyl ...	194	C11H14O3	013183-17-0	64
5			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64



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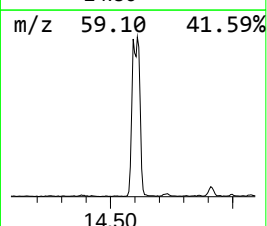
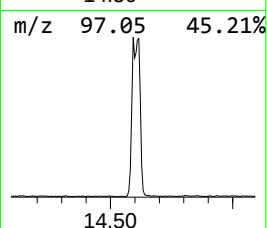
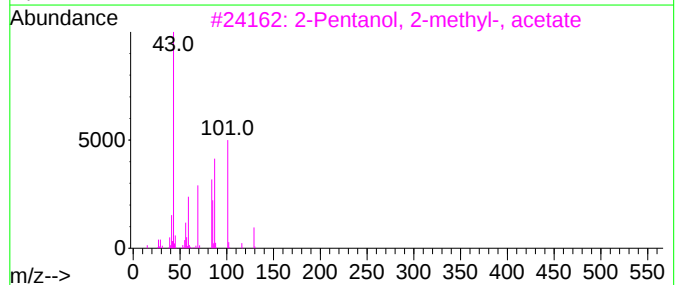
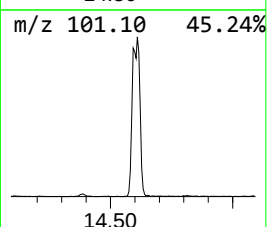
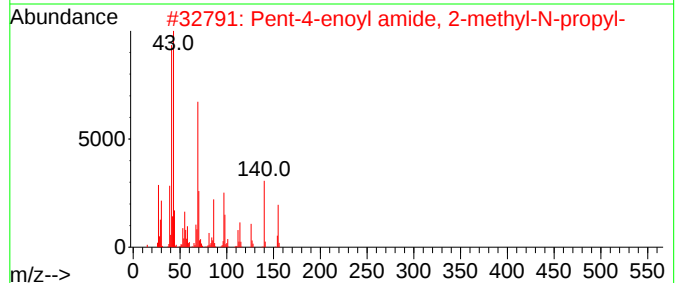
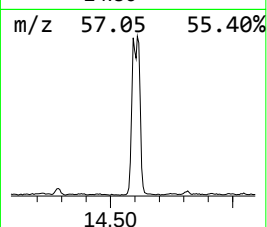
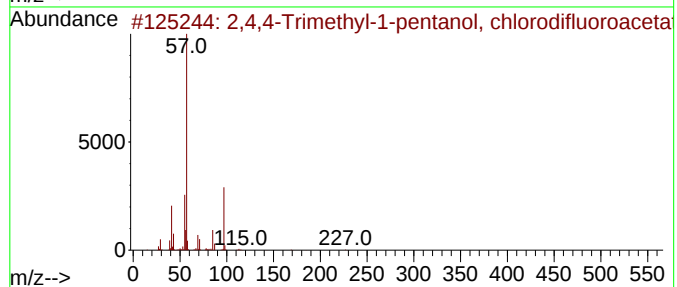
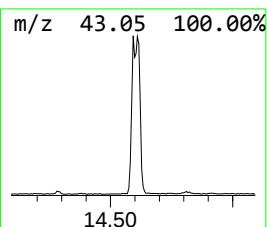
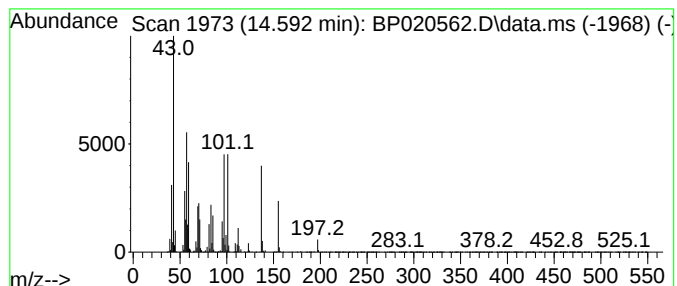
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown14.592 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.592	5.42 ng	992045	Acenaphthene-d10	14.387

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4-Trimethyl-1-pentanol, chlo...	242	C10H17ClF2O2	1000447-27-2	10		
2	Pent-4-enoyl amide, 2-methyl-N-p...	155	C9H17NO	1000420-35-2	10		
3	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10		
4	11-Tricosene	322	C23H46	052078-56-5	10		
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10		



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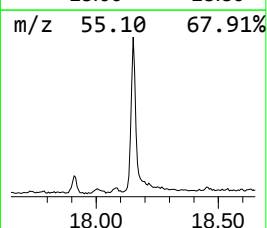
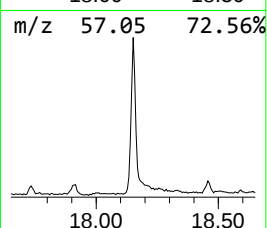
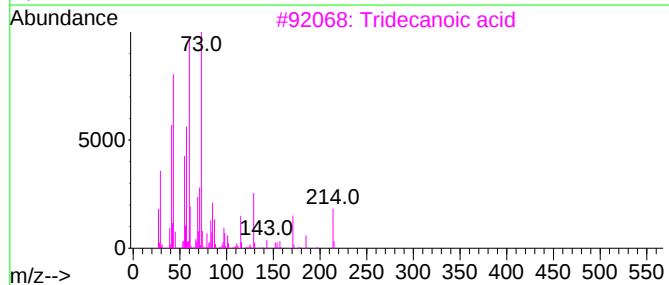
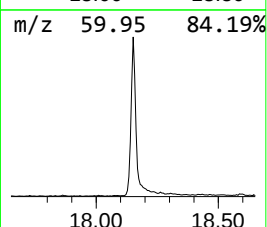
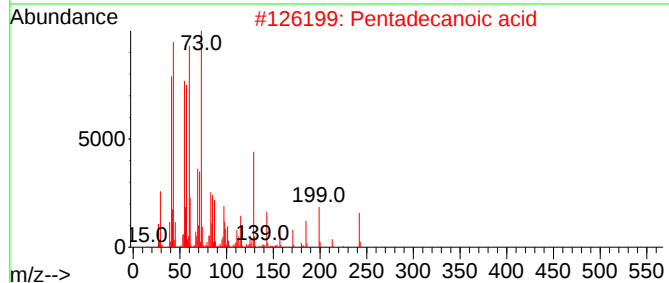
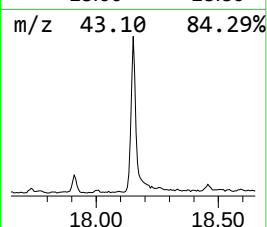
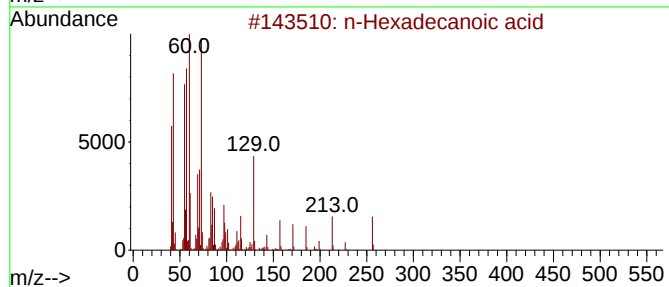
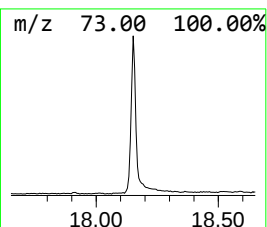
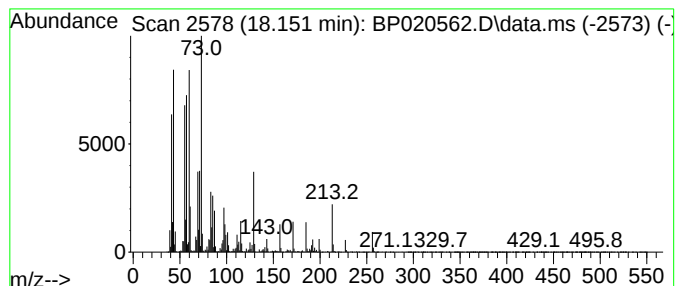
Instrument :
BNA_P
ClientSampleId :
SW-03

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.	
18.151	6.17 ng	1333860	Phenanthrene-d10		17.192	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid		256	C16H32O2	000057-10-3	99
2	Pentadecanoic acid		242	C15H30O2	001002-84-2	91
3	Tridecanoic acid		214	C13H26O2	000638-53-9	90
4	Tetradecanoic acid		228	C14H28O2	000544-63-8	72
5	8-Methylnonanoic acid		172	C10H20O2	005963-14-4	55



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
Data File : BP020562.D
Acq On : 07 Jun 2024 16:14
Operator : MA/JU
Sample : P2707-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-03

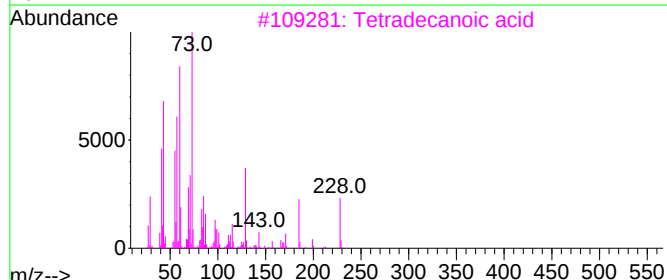
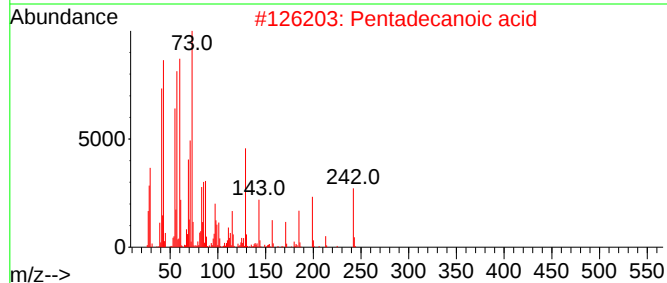
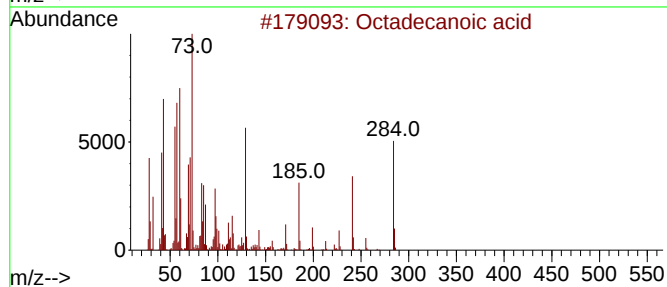
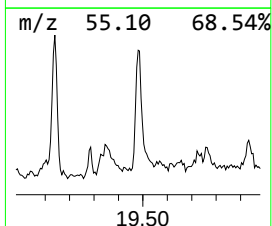
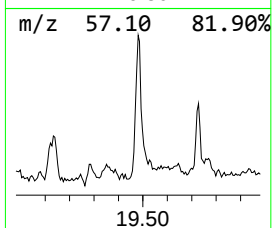
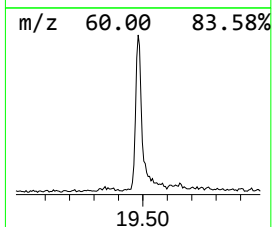
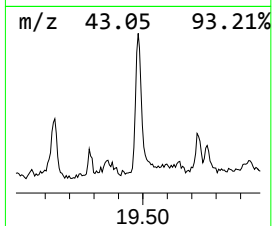
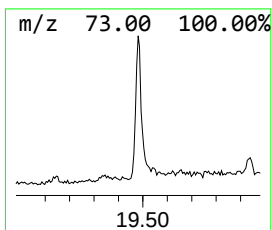
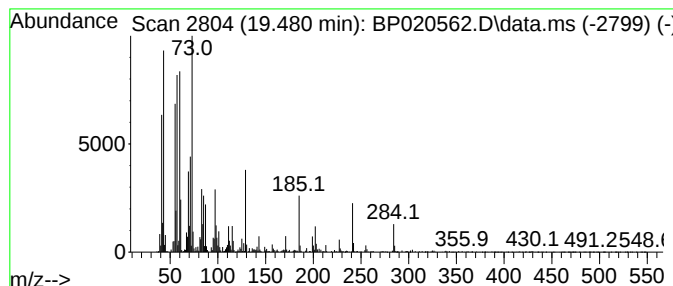
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.480	2.13 ng	532517	Chrysene-d12	21.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5			8-Methylnonanoic acid	172	C10H20O2	005963-14-4	78



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
Data File : BP020562.D
Acq On : 07 Jun 2024 16:14
Operator : MA/JU
Sample : P2707-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-03

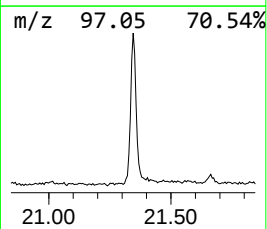
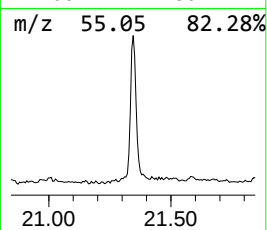
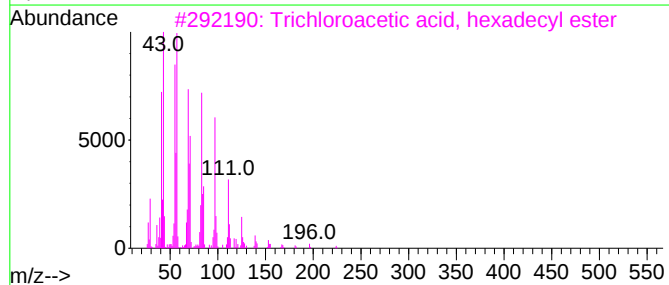
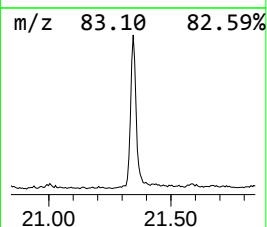
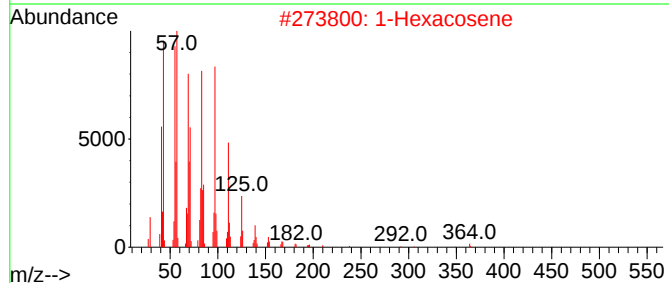
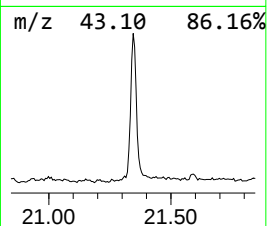
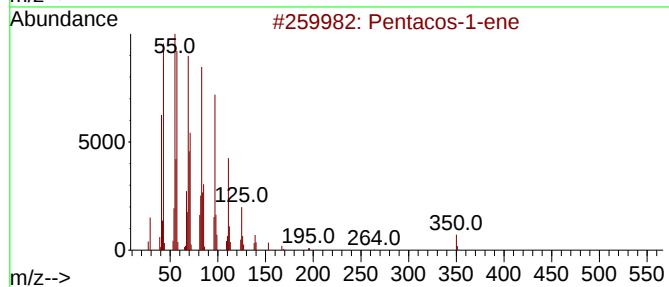
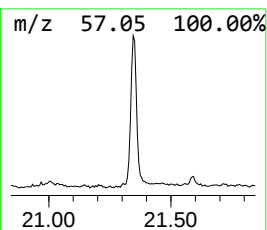
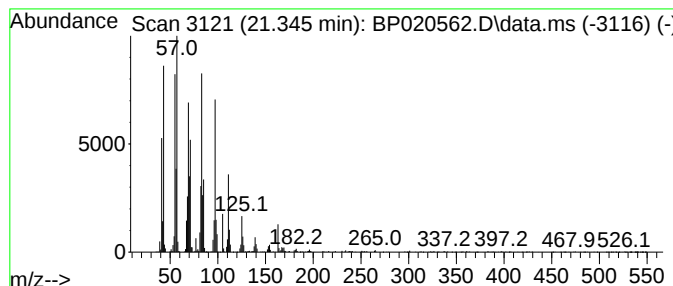
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Pentacos-1-ene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.345	4.89 ng	1224120	Chrysene-d12	21.663

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacos-1-ene	350	C25H50	016980-85-1	95
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
4			Behenic alcohol	326	C22H46O	000661-19-8	93
5			1-Heneicosanol	312	C21H44O	015594-90-8	93



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060724\
Data File : BP020562.D
Acq On : 07 Jun 2024 16:14
Operator : MA/JU
Sample : P2707-05
Misc :
ALS Vial : 10 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
SW-03

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...	3.028	28.4	ng	2906290	1	7.752	2050190	20.0
Isopropyl Alcohol	3.552	5.9	ng	601581	1	7.752	2050190	20.0
Ethanol, 2-(2-e...	7.358	3.1	ng	316920	1	7.752	2050190	20.0
1-Phenoxypropan...	11.263	3.8	ng	534177	2	10.528	2780190	20.0
unknown14.592	14.592	5.4	ng	992045	3	14.387	3659000	20.0
n-Hexadecanoic ...	18.151	6.2	ng	1333860	4	17.192	4325840	20.0
Octadecanoic acid	19.480	2.1	ng	532517	5	21.663	5009360	20.0
Pentacos-1-ene	21.345	4.9	ng	1224120	5	21.663	5009360	20.0