

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
 Data File : BP020508.D
 Acq On : 04 Jun 2024 23:23
 Operator : MA/JU
 Sample : P2687-04
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 72-11977

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: BP020508.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.040	4	9	27	rVB	2029480	3093173	27.44%	4.535%
2	3.558	93	97	111	rBV	263681	380597	3.38%	0.558%
3	5.381	399	407	417	rBV	3125591	4748051	42.11%	6.962%
4	6.928	662	670	681	rBV	3261214	5127367	45.48%	7.518%
5	7.764	804	812	819	rBV	1028170	1627994	14.44%	2.387%
6	8.911	999	1007	1018	rBV	1946066	3300395	29.27%	4.839%
7	9.463	1093	1101	1112	rVB	87271	140765	1.25%	0.206%
8	10.534	1274	1283	1293	rBV	1356157	2329824	20.67%	3.416%
9	11.269	1402	1408	1420	rBV	194774	334895	2.97%	0.491%
10	12.993	1693	1701	1710	rBV	4848161	7868422	69.79%	11.537%
11	14.387	1931	1938	1945	rBV	2088233	3124252	27.71%	4.581%
12	15.898	2188	2195	2205	rBV	3908273	5707582	50.63%	8.369%
13	17.192	2408	2415	2420	rBV	2437030	3684698	32.68%	5.403%
14	17.239	2420	2423	2428	rVB	195523	275644	2.44%	0.404%
15	18.145	2572	2577	2586	rBV2	360464	557713	4.95%	0.818%
16	19.328	2772	2778	2784	rBV	443951	691691	6.14%	1.014%
17	19.475	2799	2803	2817	rVB2	171001	275715	2.45%	0.404%
18	19.698	2834	2841	2850	rVB	328646	554205	4.92%	0.813%
19	19.928	2874	2880	2891	rVB	7954191	11274085	100.00%	16.531%
20	21.333	3115	3119	3133	rVB3	404453	831167	7.37%	1.219%
21	21.586	3157	3162	3166	rBV	1138159	1520708	13.49%	2.230%
22	21.645	3166	3172	3178	rVV2	2329520	3868668	34.31%	5.673%
23	22.963	3390	3396	3402	rBV	1344793	2576944	22.86%	3.778%
24	23.433	3473	3476	3482	rVB2	170550	262437	2.33%	0.385%
25	24.998	3733	3742	3754	rVB	1440715	4043410	35.86%	5.929%

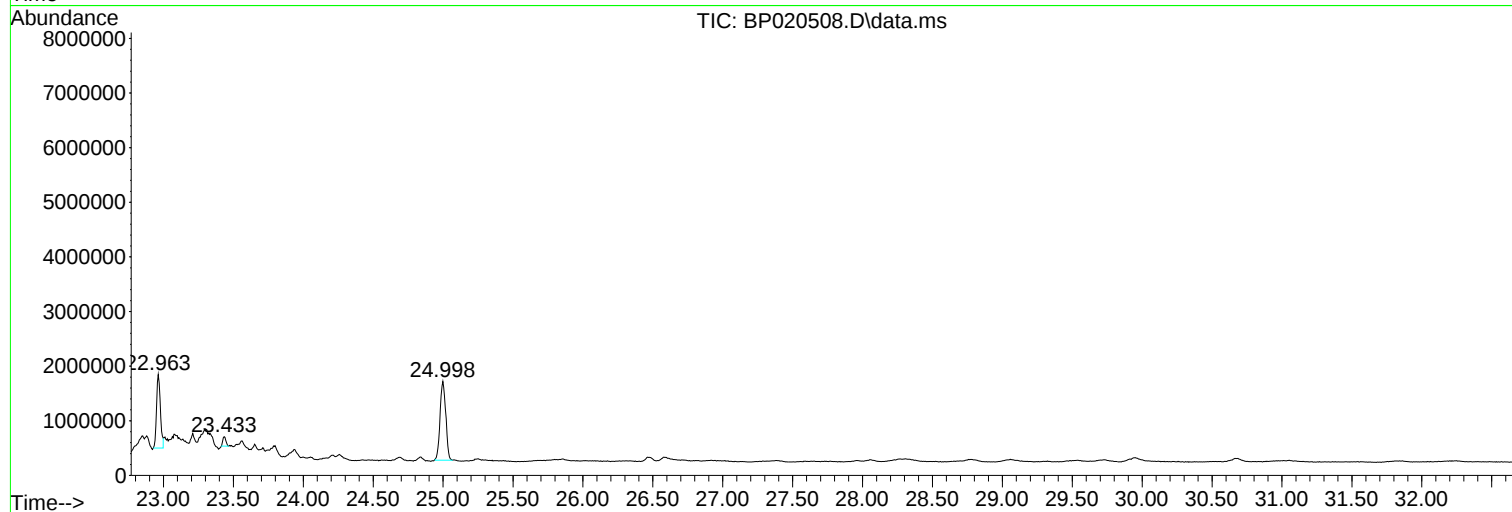
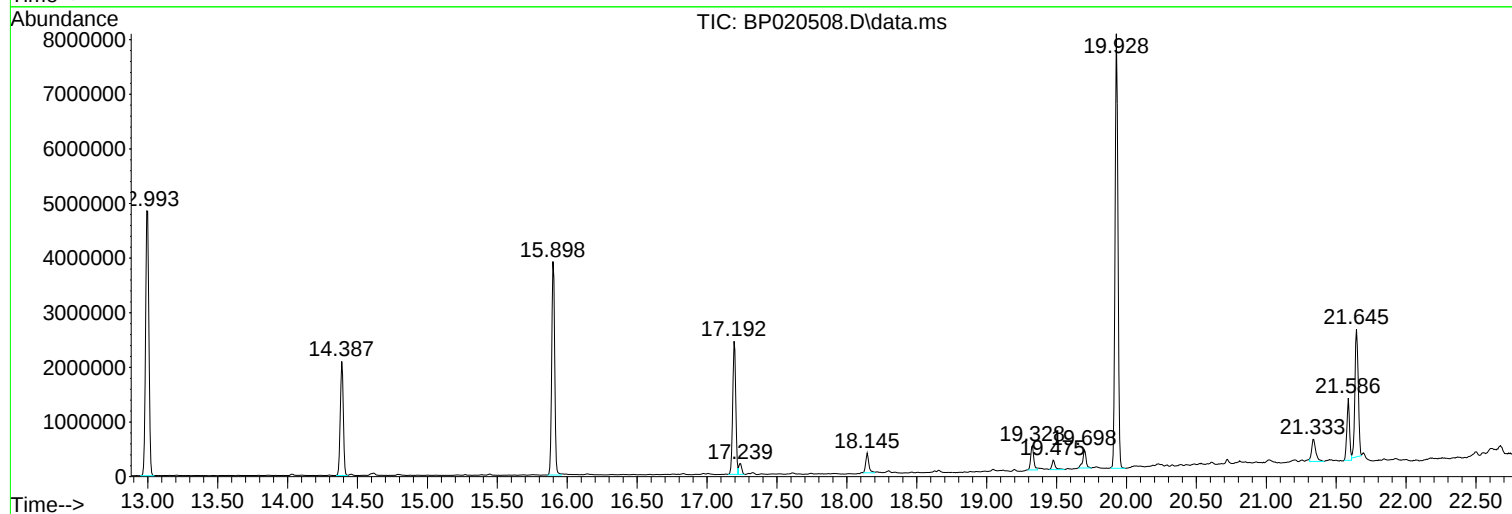
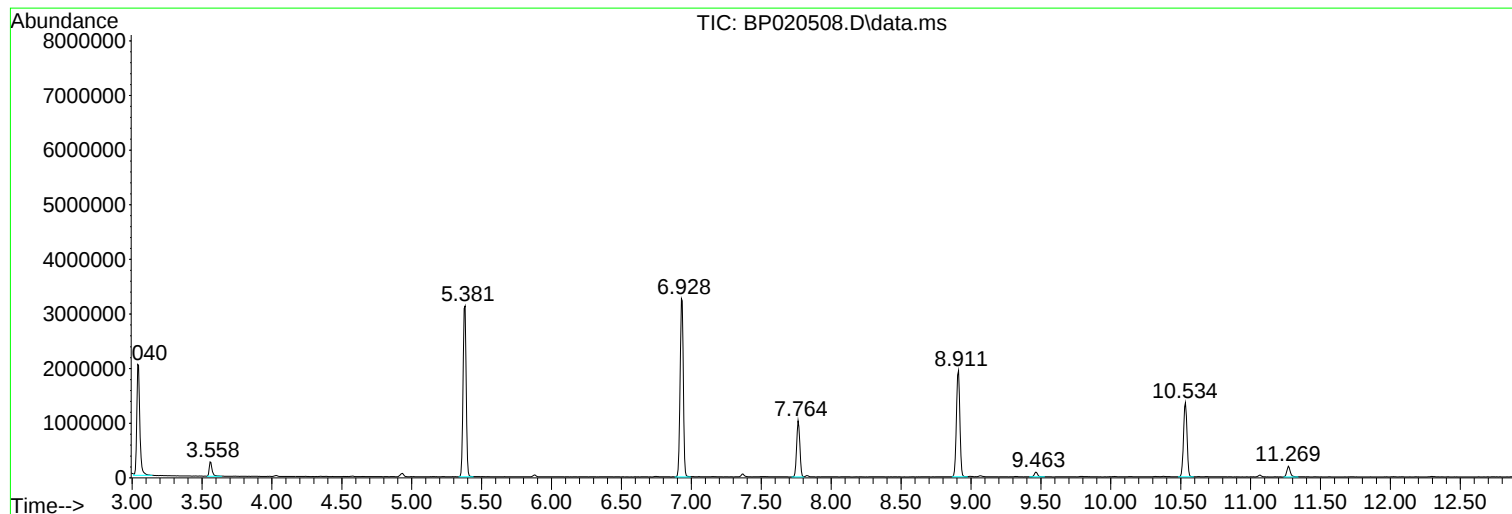
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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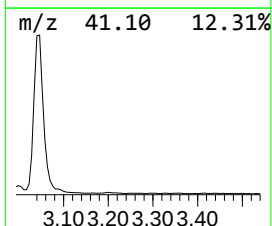
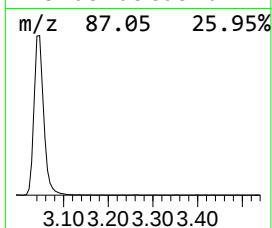
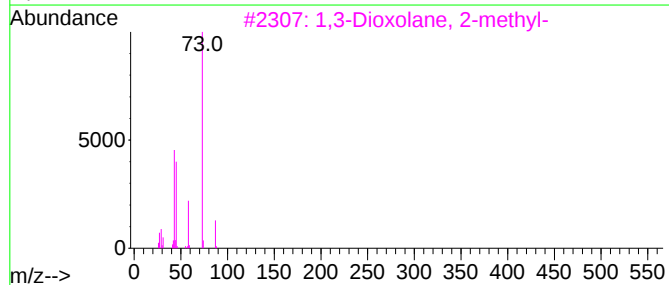
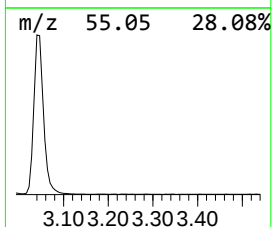
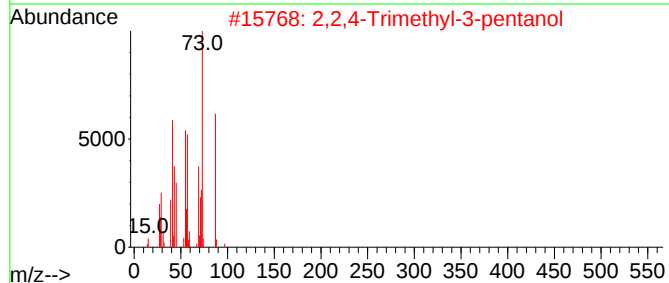
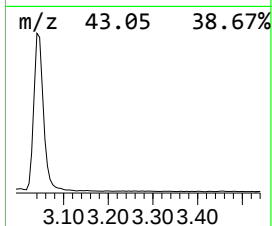
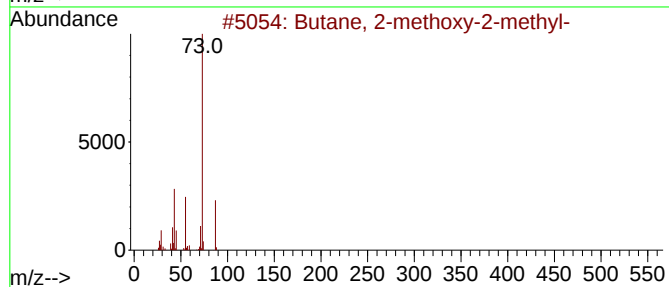
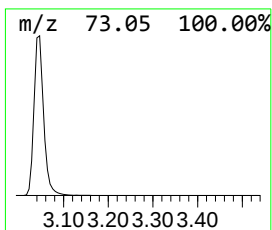
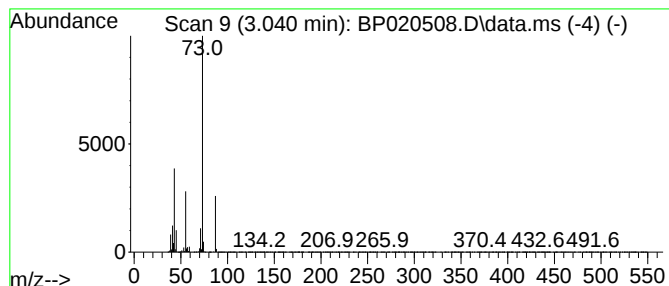
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
3.040	38.00 ng	3093170	1,4-Dichlorobenzene-d4	7.764

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			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	27
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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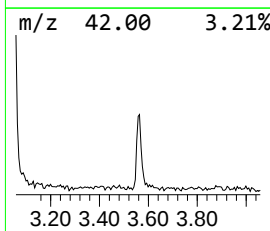
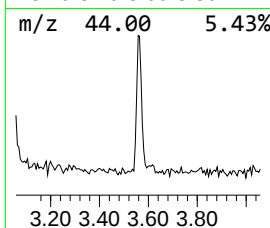
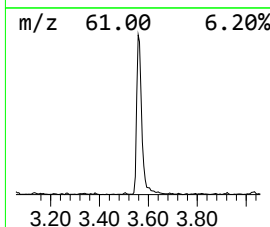
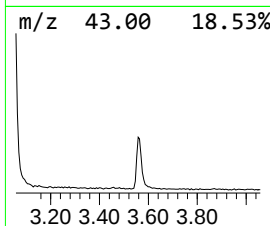
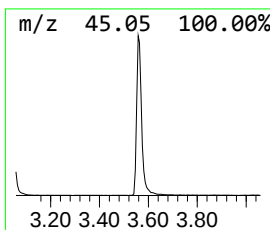
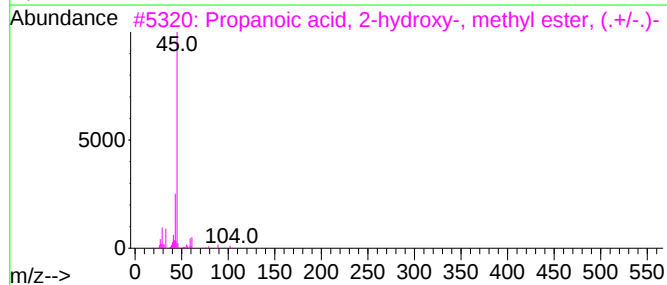
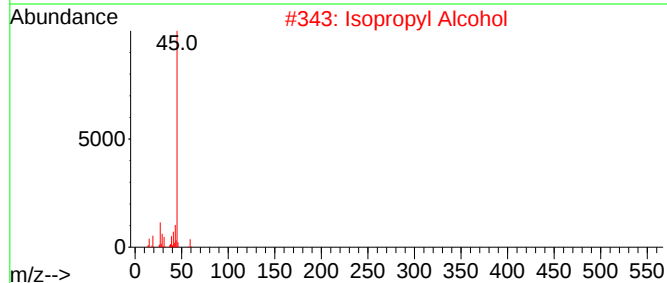
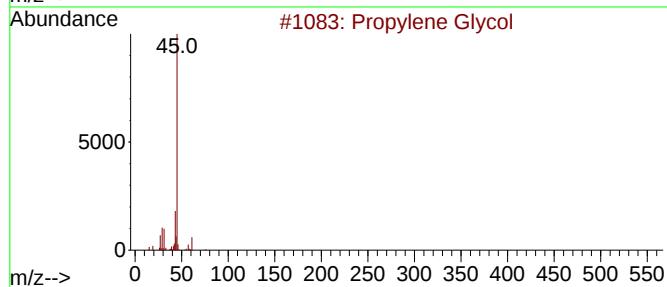
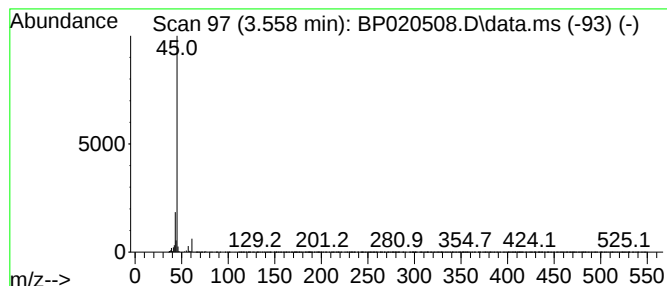
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propylene Glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.558	4.68 ng	380597	1,4-Dichlorobenzene-d4	7.764

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propylene Glycol	76	C3H8O2	000057-55-6	90
2			Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3			Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4			R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9
5			(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9



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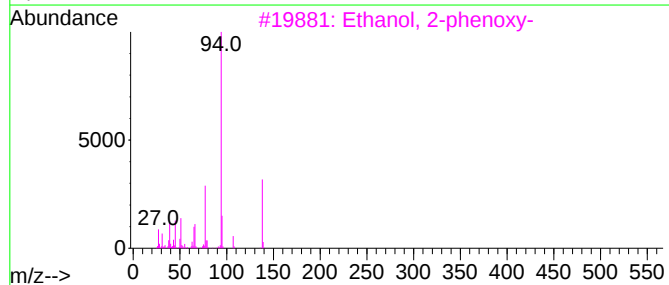
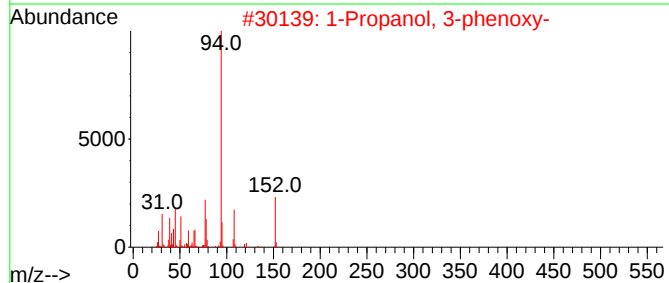
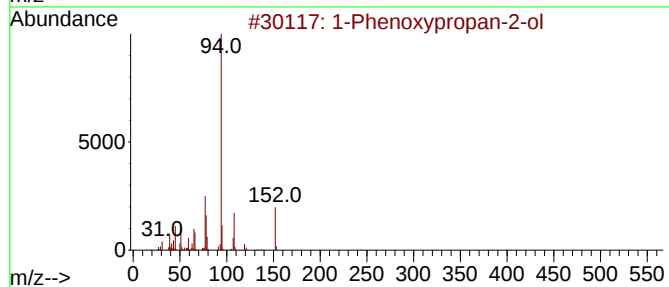
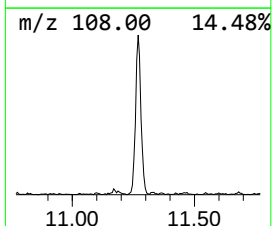
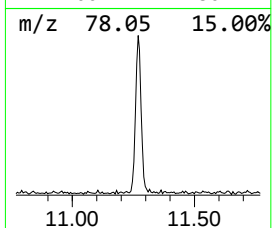
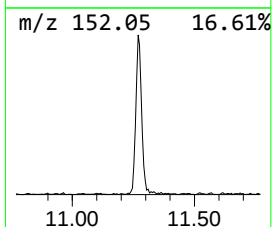
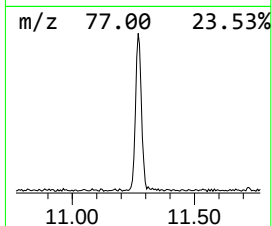
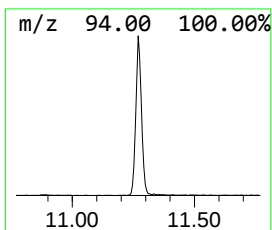
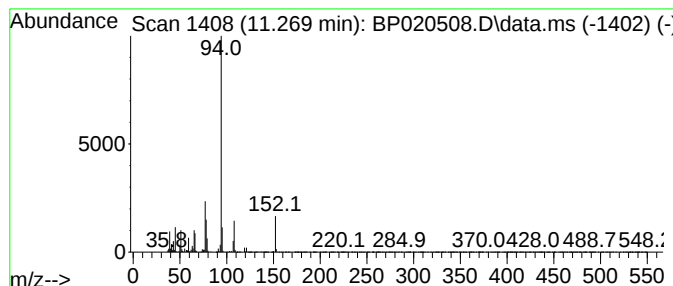
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.269	2.87 ng	334895	Naphthalene-d8	10.534

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	90
3			Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
4			Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5			1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64



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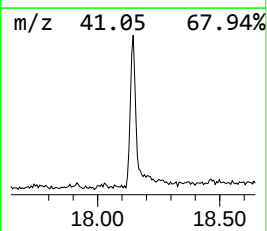
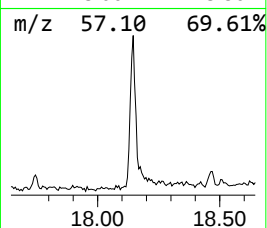
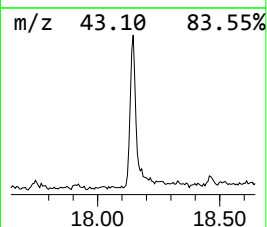
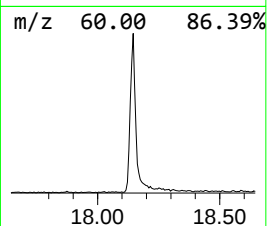
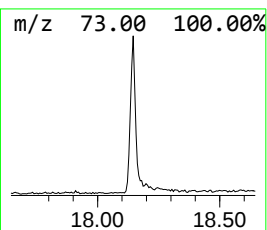
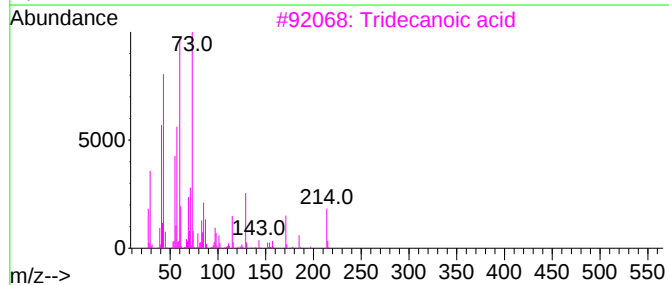
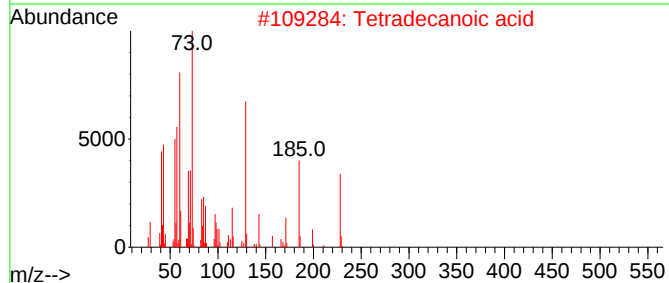
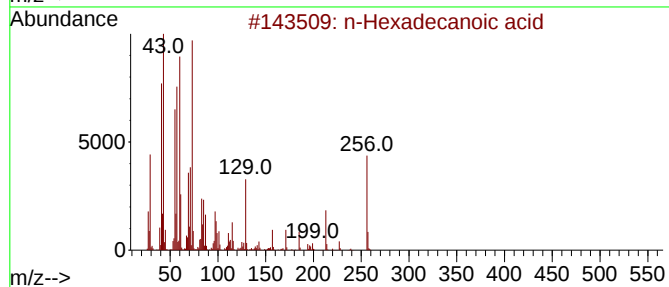
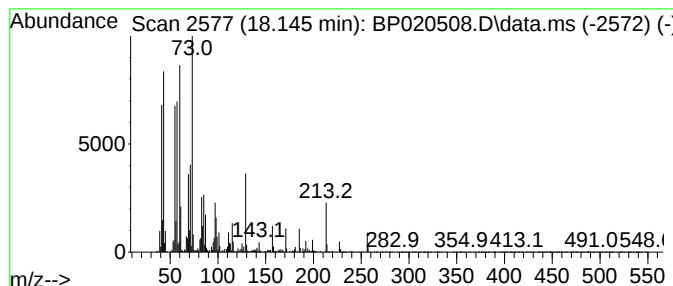
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Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.145	3.03 ng	557713	Phenanthrene-d10	17.192

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	90
3		Tridecanoic acid	214	C13H26O2	000638-53-9	87
4		Octadecanoic acid	284	C18H36O2	000057-11-4	87
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	81



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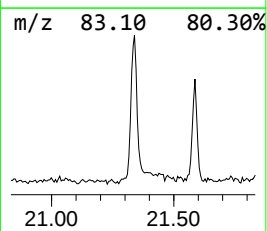
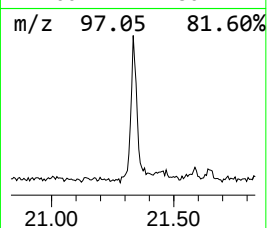
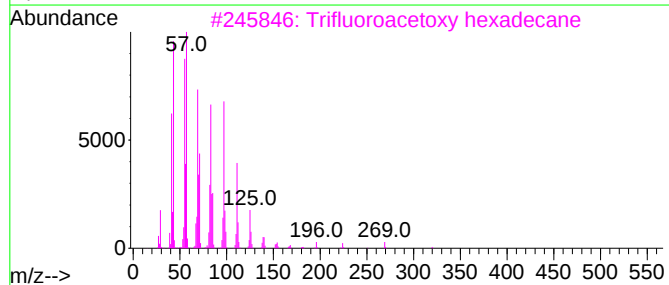
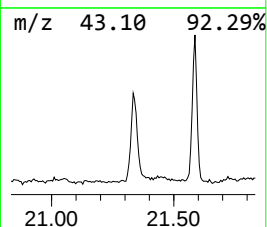
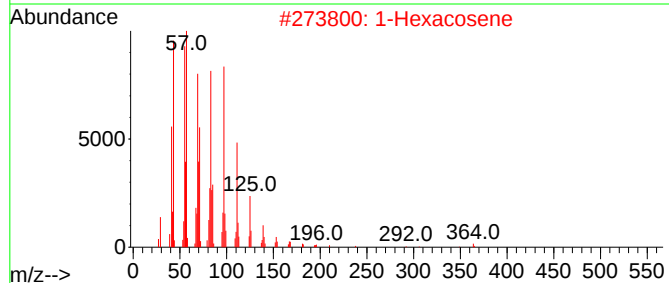
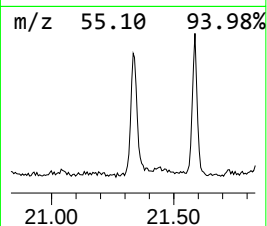
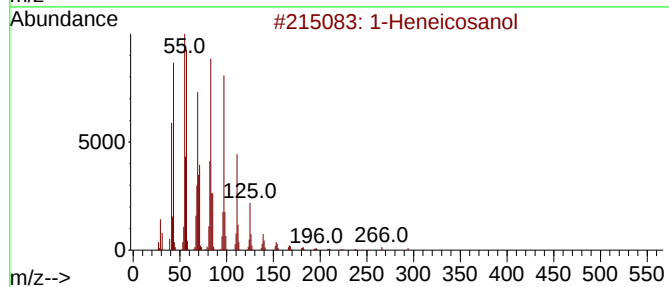
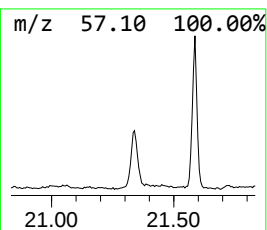
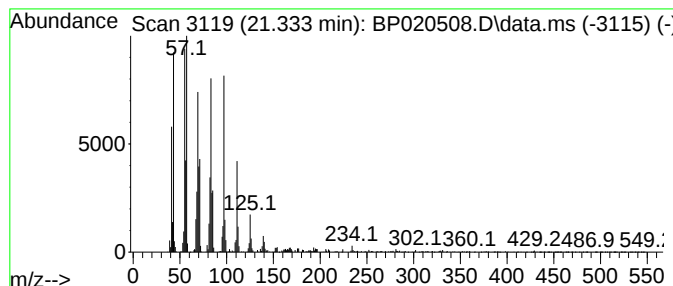
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.333	4.30 ng	831167	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	94
2			1-Hexacosene	364	C26H52	018835-33-1	94
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
4			Heptacos-1-ene	378	C27H54	015306-27-1	94
5			1-Nonadecene	266	C19H38	018435-45-5	91



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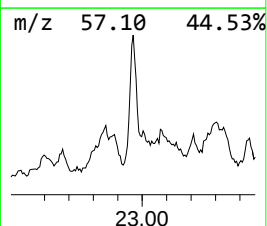
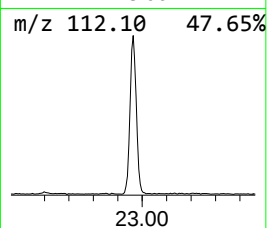
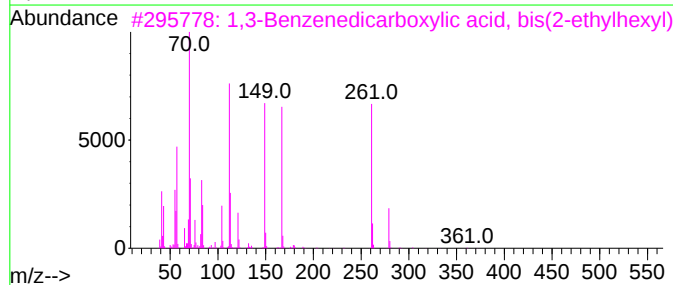
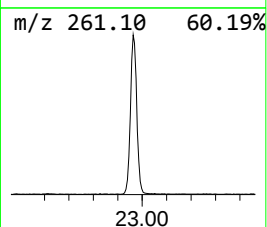
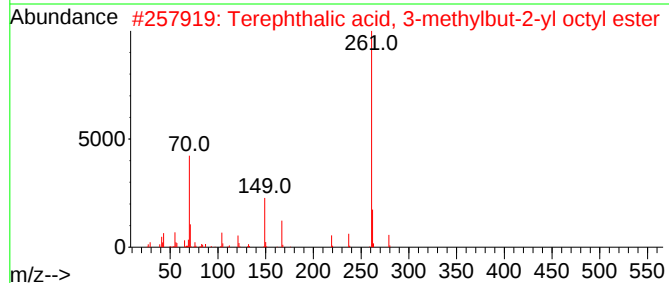
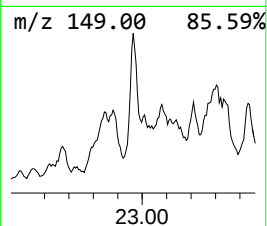
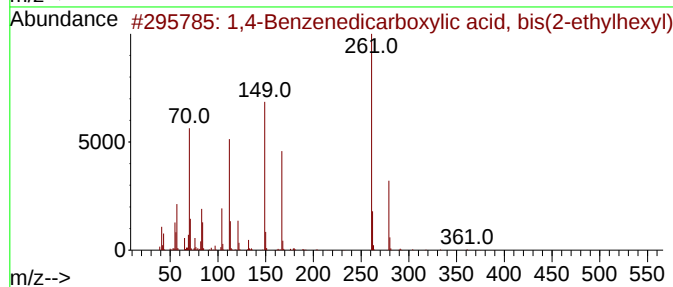
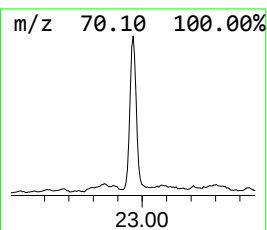
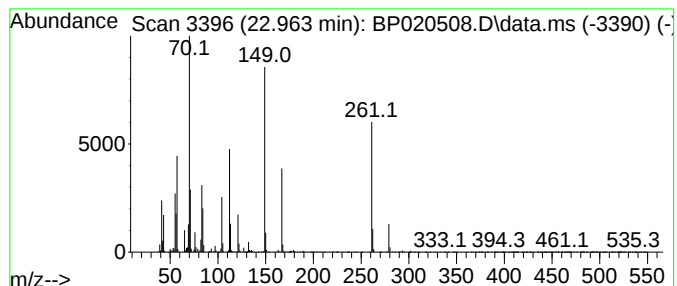
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP052924.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 1,4-Benzenedicarboxylic aci... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.963	13.32 ng	2576940	Chrysene-d12	21.645

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Benzenedicarboxylic acid, bi...	390	C24H38O4	006422-86-2	87
2			Terephthalic acid, 3-methylbut-2...	348	C21H32O4	1000356-27-6	64
3			1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	59
4			Isophthalic acid, 3-methylbut-2...	348	C21H32O4	1000344-72-4	47
5			Terephthalic acid, monochloride,...	296	C16H21ClO3	1000324-22-9	43



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP060424\
Data File : BP020508.D
Acq On : 04 Jun 2024 23:23
Operator : MA/JU
Sample : P2687-04
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
72-11977

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	3.040	38.0	ng	3093170	1	7.764	1627990	20.0
Propylene Glycol	3.558	4.7	ng	380597	1	7.764	1627990	20.0
1-Phenoxypropan...	11.269	2.9	ng	334895	2	10.534	2329820	20.0
n-Hexadecanoic ...	18.145	3.0	ng	557713	4	17.192	3684700	20.0
1-Heneicosanol	21.333	4.3	ng	831167	5	21.645	3868670	20.0
1,4-Benzenedica...	22.963	13.3	ng	2576940	5	21.645	3868670	20.0