

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030722\
 Data File : BP009295.D
 Acq On : 07 Mar 2022 20:43
 Operator : CG/JU
 Sample : N1727-01
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 20220215-096-21-03-ELUTRIATE

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-BP030522.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP009295.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.075	11	15	32	rVB	2860272	4580457	22.48%	3.329%
2	5.416	406	413	423	rBV	4692489	7485679	36.74%	5.441%
3	6.987	673	680	692	rBV	3175954	5787388	28.40%	4.207%
4	7.822	812	822	829	rBV	1786976	3084796	15.14%	2.242%
5	7.893	829	834	843	rVB	167334	281792	1.38%	0.205%
6	8.975	1004	1018	1028	rBV	4914413	8789510	43.14%	6.389%
7	9.446	1090	1098	1105	rVB	156666	286439	1.41%	0.208%
8	10.399	1251	1260	1271	rBV	699383	1166469	5.72%	0.848%
9	10.616	1288	1297	1305	rBV	2302185	4156763	20.40%	3.021%
10	13.081	1709	1716	1727	rVB	12376636	19624575	96.31%	14.264%
11	13.304	1749	1754	1761	rBV	169073	248704	1.22%	0.181%
12	14.457	1943	1950	1958	rBV	3333372	5191271	25.48%	3.773%
13	14.687	1983	1989	1993	rBV	173993	242767	1.19%	0.176%
14	15.951	2198	2204	2213	rVB	9388372	13966701	68.55%	10.152%
15	17.216	2413	2419	2428	rBV	3727620	5761033	28.27%	4.187%
16	17.292	2428	2432	2435	rBV	153510	225942	1.11%	0.164%
17	17.522	2465	2471	2483	rVB	14715828	20375692	100.00%	14.810%
18	17.910	2532	2537	2545	rVB	625290	892569	4.38%	0.649%
19	18.122	2569	2573	2579	rBV	427331	622699	3.06%	0.453%
20	19.051	2727	2731	2739	rVB	474226	614679	3.02%	0.447%
21	19.792	2852	2857	2864	rVB	14154292	19418458	95.30%	14.114%
22	21.051	3067	3071	3079	rBV	1246270	1801273	8.84%	1.309%
23	21.327	3112	3118	3125	rVB	4360509	6219415	30.52%	4.521%
24	23.733	3520	3527	3541	rVB2	3093186	6755864	33.16%	4.910%

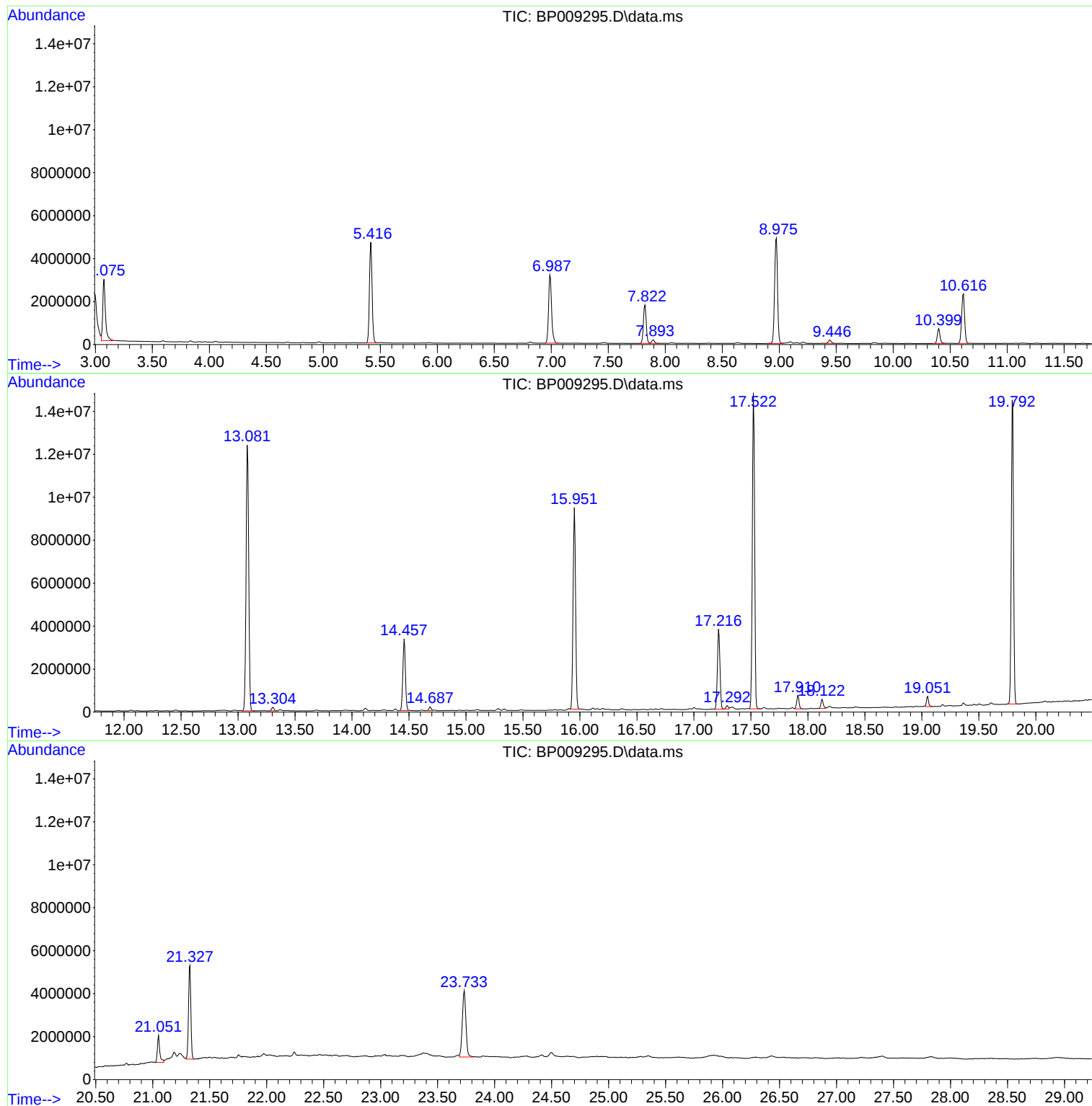
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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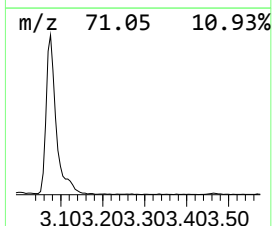
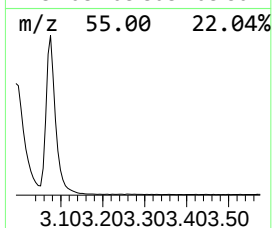
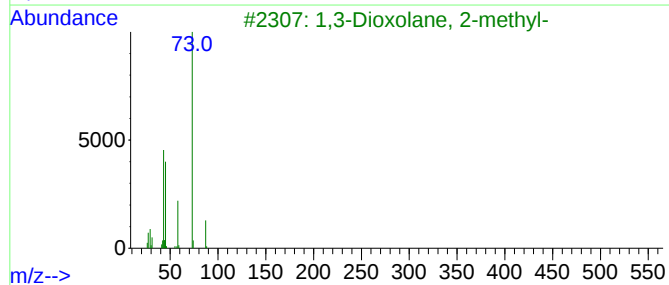
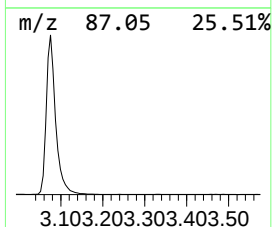
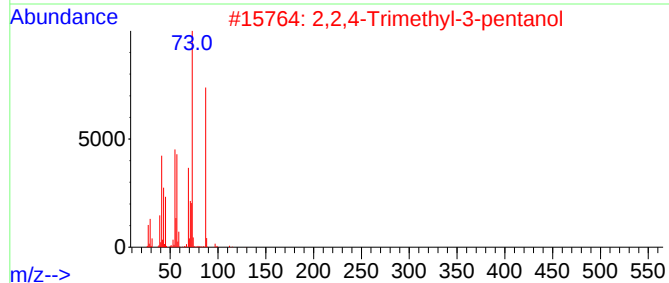
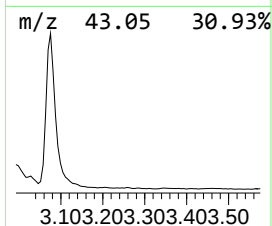
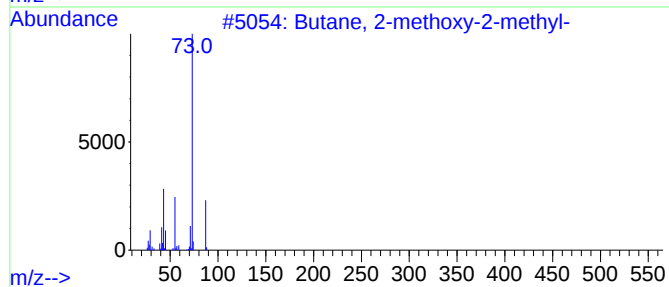
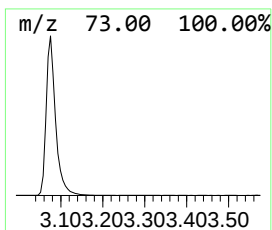
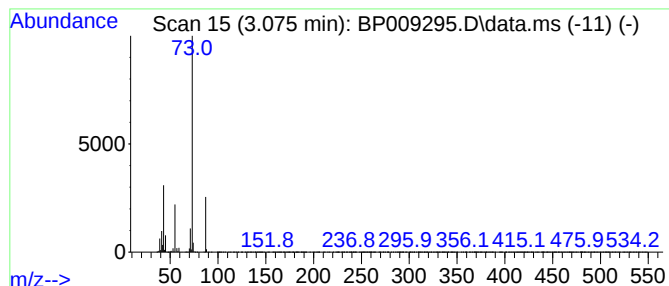
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.075	29.70 ng	4580460	1,4-Dichlorobenzene-d4	7.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	90
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	43
3			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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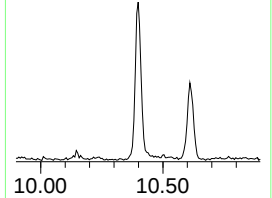
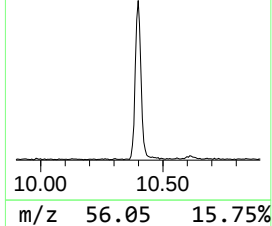
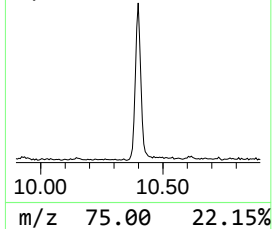
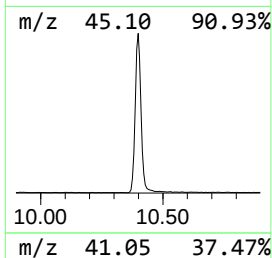
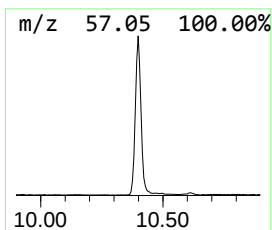
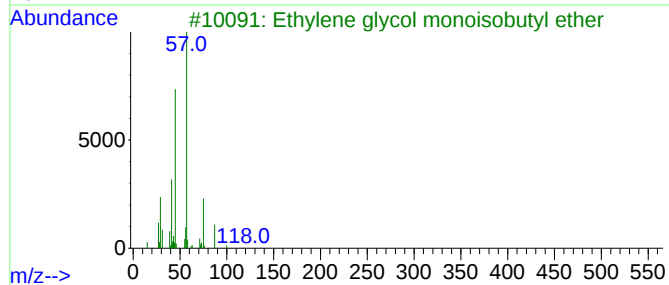
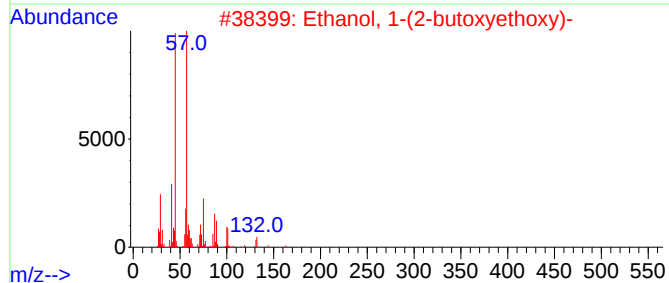
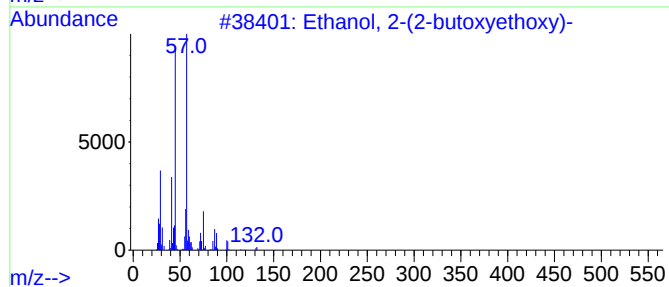
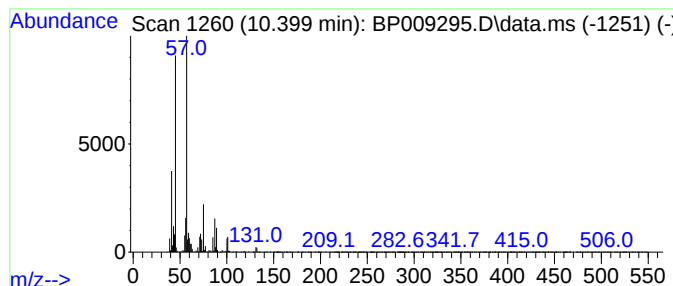
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.399	5.61 ng	1166470	Naphthalene-d8	10.616

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	90
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	83
3			Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	64
4			3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	50
5			Methoxyacetic acid, 2-butyl ester	146	C7H14O3	070159-90-9	50



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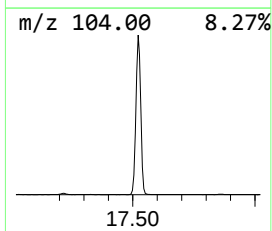
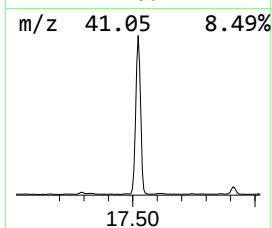
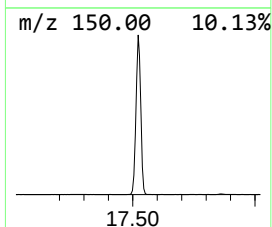
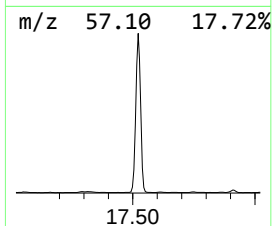
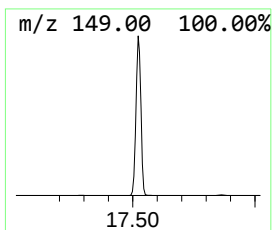
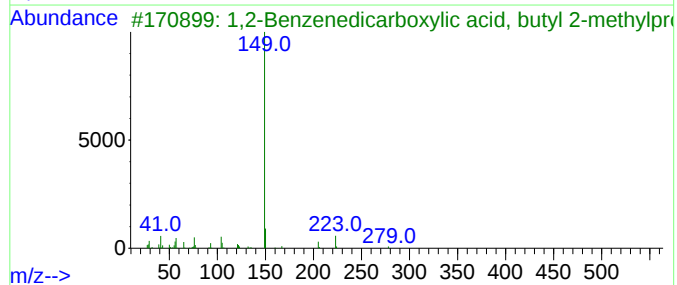
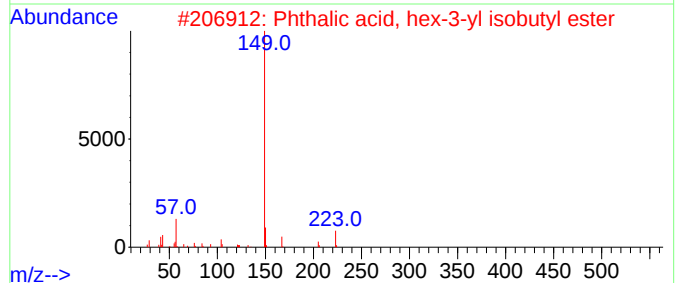
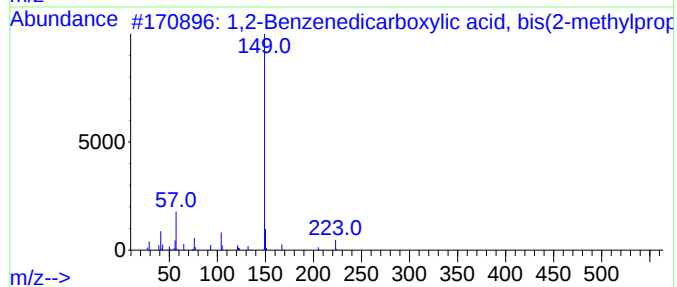
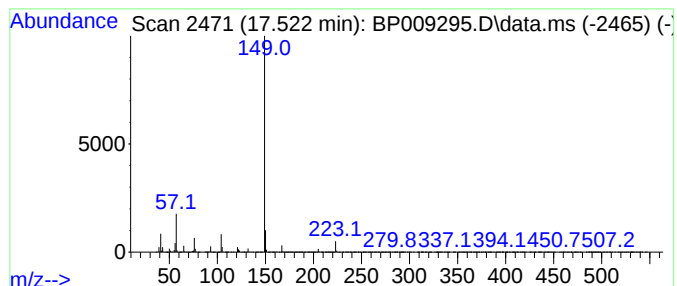
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Peak Number 3 1,2-Benzenedicarboxylic aci... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.522	70.74 ng	20375700	Phenanthrene-d10	17.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	91
2			Phthalic acid, hex-3-yl isobutyl...	306	C18H26O4	1000356-95-4	86
3			1,2-Benzenedicarboxylic acid, bu...	278	C16H22O4	017851-53-5	86
4			Phthalic acid, decyl isobutyl ester	362	C22H34O4	1000308-94-2	83
5			Phthalic acid, isobutyl nonyl ester	348	C21H32O4	1000309-04-4	83



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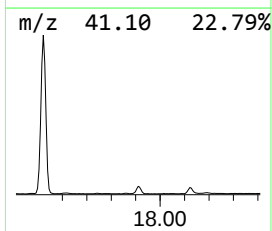
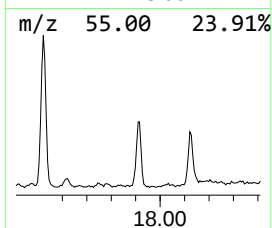
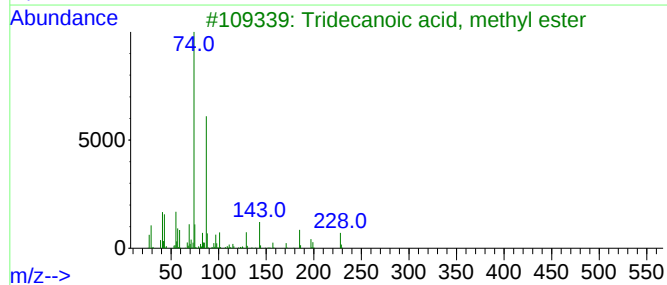
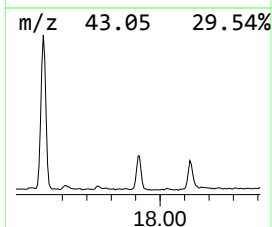
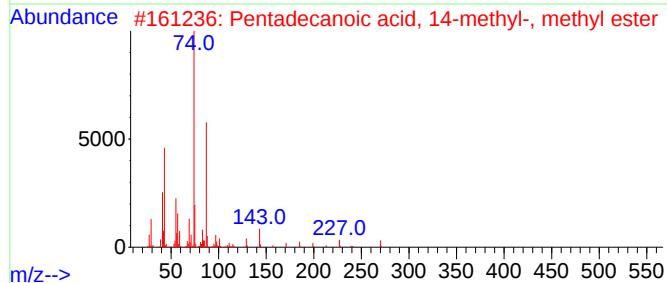
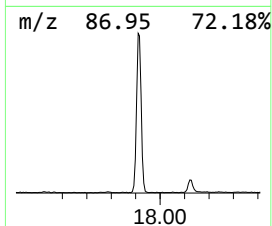
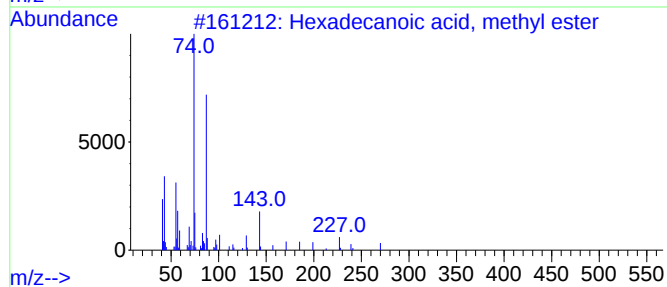
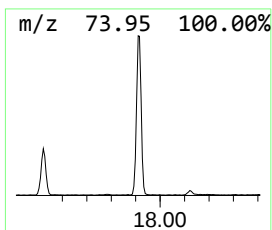
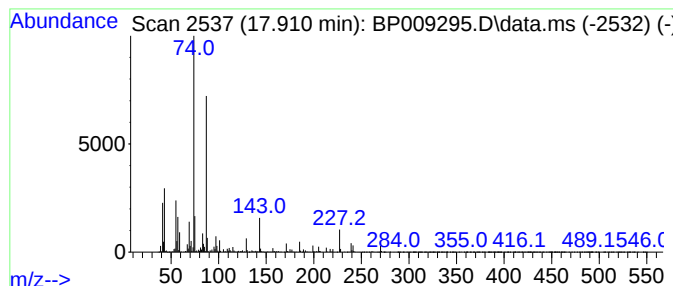
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.910	3.10 ng	892569	Phenanthrene-d10	17.216

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2			Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	97
3			Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	87
4			Methyl tetradecanoate	242	C15H30O2	000124-10-7	83
5			Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	80



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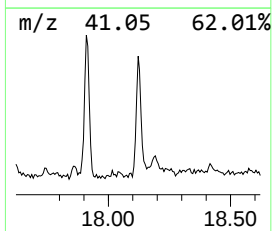
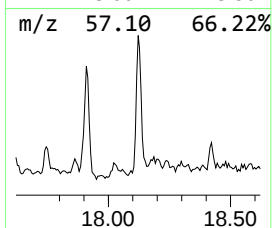
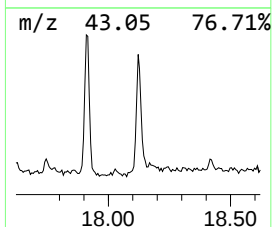
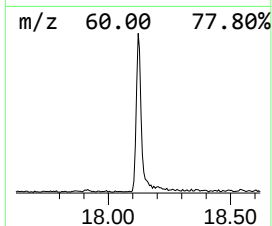
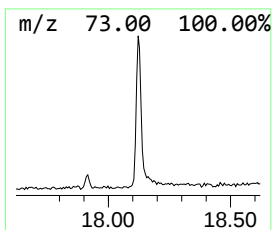
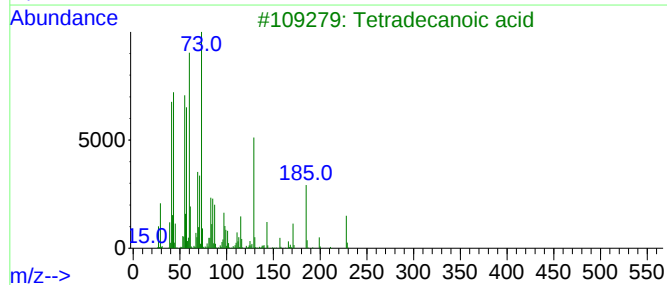
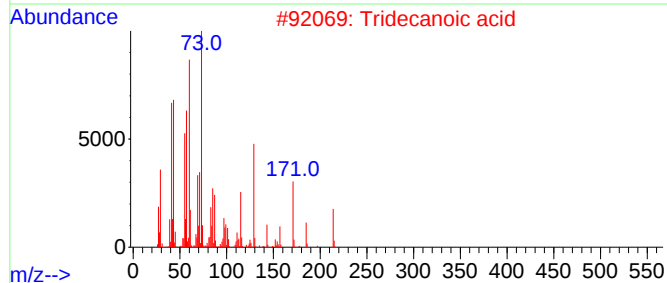
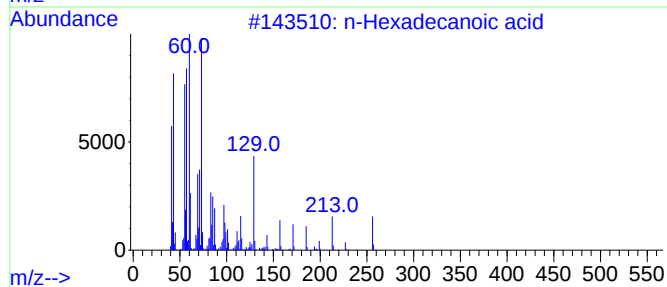
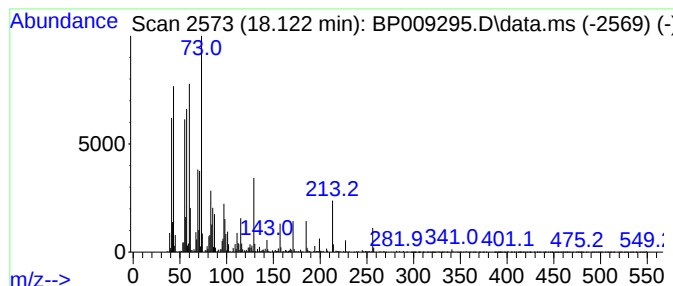
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.122	2.16 ng	622699	Phenanthrene-d10	17.216

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	83
4			Octadecanoic acid	284	C18H36O2	000057-11-4	81
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	68



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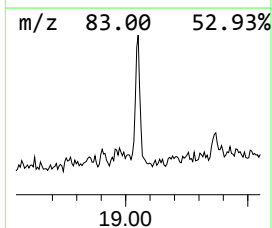
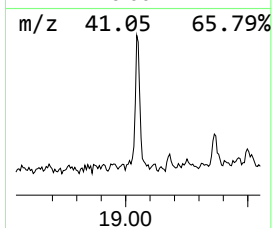
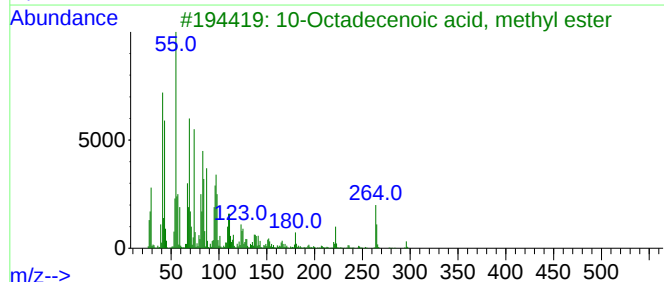
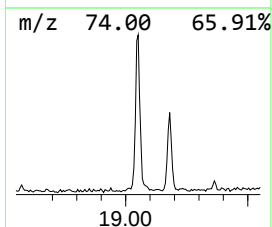
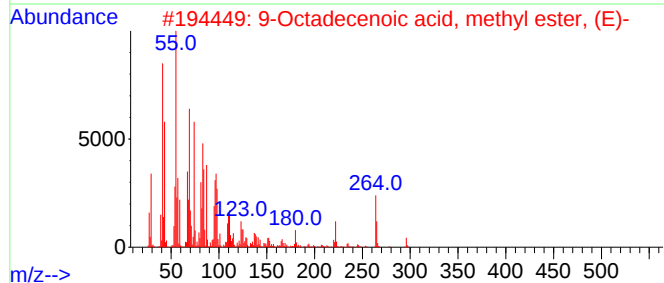
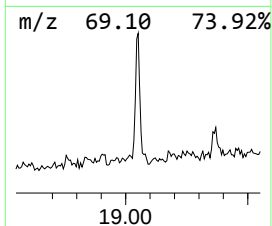
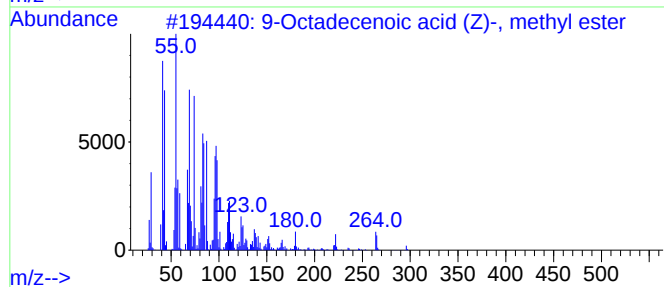
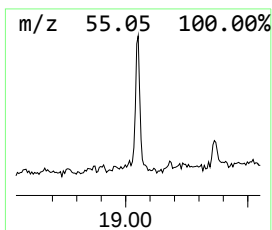
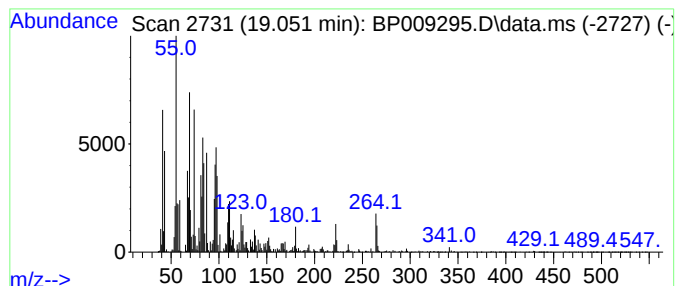
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BNA_P
ClientSampleId :
20220215-096-21-03-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 9-Octadecenoic acid (Z)-, m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.051	2.13 ng	614679	Phenanthrene-d10	17.216	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
2	9-Octadecenoic acid, methyl este...	296	C19H36O2	001937-62-8	99
3	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
4	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	99
5	9-Octadecenoic acid, methyl ester	296	C19H36O2	002462-84-2	99



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030722\
Data File : BP009295.D
Acq On : 07 Mar 2022 20:43
Operator : CG/JU
Sample : N1727-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220215-096-21-03-ELUTRIATE

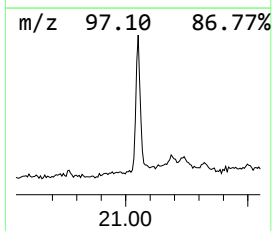
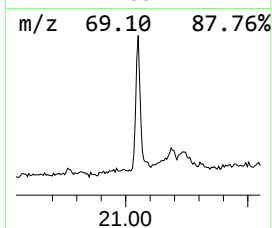
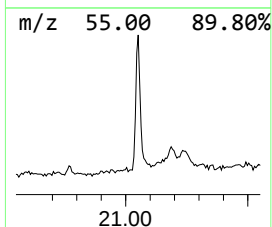
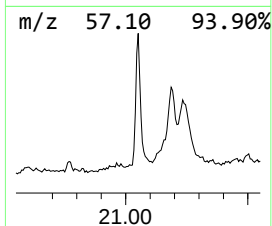
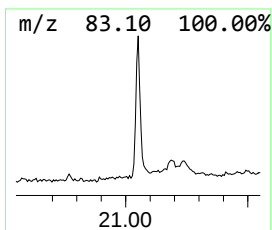
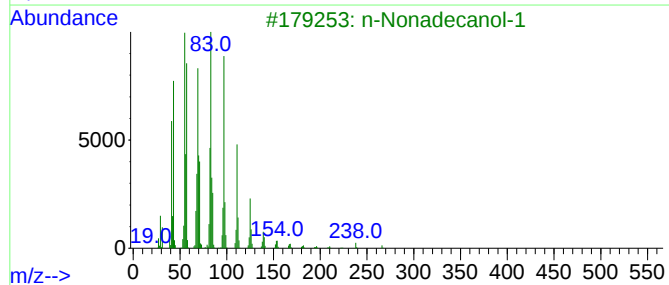
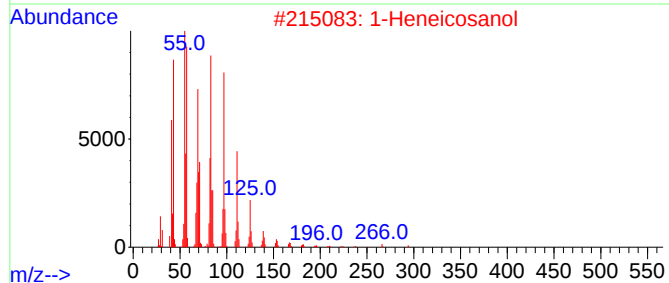
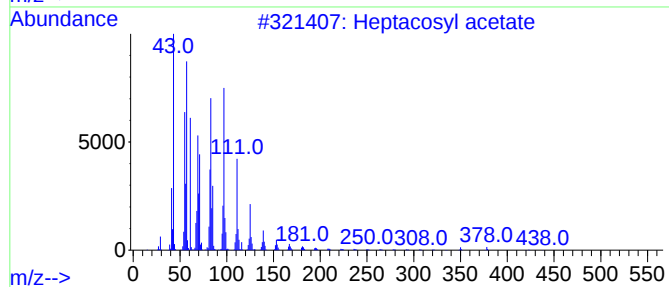
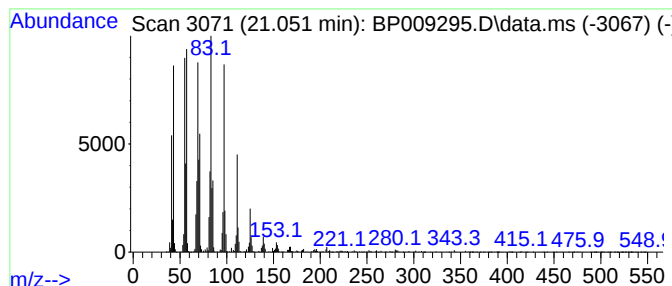
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptacosyl acetate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.051	5.79 ng	1801270	Chrysene-d12	21.327

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	96
2			1-Heneicosanol	312	C21H44O	015594-90-8	95
3			n-Nonadecanol-1	284	C19H40O	001454-84-8	94
4			Heptacos-1-ene	378	C27H54	015306-27-1	94
5			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP030722\
Data File : BP009295.D
Acq On : 07 Mar 2022 20:43
Operator : CG/JU
Sample : N1727-01
Misc :
ALS Vial : 17 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
20220215-096-21-03-ELUTRIATE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP030522.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...	3.075	29.7	ng	4580460	1	7.822	3084800	20.0
Ethanol, 2-(2-b...	10.399	5.6	ng	1166470	2	10.616	4156760	20.0
1,2-Benzenedica...	17.522	70.7	ng	20375700	4	17.216	5761030	20.0
Hexadecanoic ac...	17.910	3.1	ng	892569	4	17.216	5761030	20.0
n-Hexadecanoic ...	18.122	2.2	ng	622699	4	17.216	5761030	20.0
9-Octadecenoic ...	19.051	2.1	ng	614679	4	17.216	5761030	20.0
Heptacosyl acetate	21.051	5.8	ng	1801270	5	21.327	6219420	20.0